

PB-239 249

OPTIMUM WORKING FLUIDS FOR AUTOMOTIVE RANKINE ENGINES.
VOLUME III. TECHNICAL SECTION APPENDICES

MONSANTO RESEARCH CORPORATION

PREPARED FOR
ENVIRONMENTAL PROTECTION AGENCY
SUNDSTRAND AVIATION

JUNE 1973

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TECHNICAL REPORT DATA (Please read instructions on the reverse before completing)		
1. REPORT NO. APTD - 1565	2.	3. PB 239 249
4. TITLE AND SUBTITLE Optimum Working Fluids for Automotive Rankine Engines Volume III - Technical Section - Appendices	5. REPORT DATE June 1973	
7. AUTHOR(S) D.R. Miller, H. R. Null, Q.E. Thompson, A.C. Pauls, J. A. Conover	6. PERFORMING ORGANIZATION CODE	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Monsanto Research Corporation 800 North Lindbergh Blvd. St. Louis, Missouri 63166	8. PERFORMING ORGANIZATION REPORT NO.	
12. SPONSORING AGENCY NAME AND ADDRESS U. S. ENVIRONMENTAL PROTECTION AGENCY Office of Mobile Source Air Pollution Control Advanced Automotive Power Systems Development Division Ann Arbor, Michigan 48105	10. PROGRAM ELEMENT NO.	
	11. CONTRACT/GRANT NO. 68 - 04 - 0030	
	13. TYPE OF REPORT AND PERIOD COVERED	
	14. SPONSORING AGENCY CODE	
15. SUPPLEMENTARY NOTES		
16. ABSTRACT The objective was to conduct a comprehensive program to establish the optimum working fluids and/ or working fluid-lubricant combinations for automotive Rankine cycle applications. The specific requirements are described and are listed as follows: (A) Vehicle Design Goals, (B) Low Temperature, (C) Materials Compatibility, (D) System Constraints, (E) Safety, (F) System Fluids Cost, (G) Stability. The tasks required for the technical effort of the contract were as follows: (1) Establish Working Fluid Selection Criteria, (2) Provide Systems Analysis, (3) Search for Existing Fluids, (4) Recommendations and Conclusions, (5) Property prediction Verification, (6) Dynamic Loop Tests, (7) Develop Preliminary Cost Estimates. This Volume III contains the technical details of the study and computer programs in appendix A through appendix Q.		
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17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution Rankine cycle Engines Design Turbines Computer programs Reciprocating Engines	Working Fluid Mixed Fluorobenzenes Aqueous Pyridines	13 B 21 G 21 E 14 B 7 C
18. DISTRIBUTION STATEMENT Release Unlimited	19. SECURITY CLASS (This Report)	21. NO. OF PAGES 252
	20. SECURITY CLASS (This page)	22. PRICE 7.50 - 2.25

APTD-1565

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VOLUME III - TECHNICAL SECTION-
APPENDICES**

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Office of Air and Water Programs
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Ann Arbor, Michigan 48105

June 1973

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APPENDIX A

SCOPE OF WORK, CONTRACT 68-04-0030

I. PURPOSE

The contractor shall conduct a comprehensive program to establish the optimum working fluids and/or working fluid-lubricant combinations for automotive Rankine cycle applications. As it is highly unlikely that the same "optimum" working fluid can be used with a reciprocating expander as with a rotary expander, a minimum of two working fluids will have to be established under this project. In addition to the establishment of an optimum reciprocating expander working fluid, a lubricant which is compatible with the working fluid is required. While utilization of the working fluid as the lubricant in the rotary expander is possible, the necessity of establishing a rotating expander lubricant is not ruled out. The contractor's selection will be based on all practical considerations with respect to emissions, safety, net cost of ownership, size, and automotive applicability.

The specific requirements and tasks required in the Scope of Work shall include but not be limited to those detailed in the following sections. All considerations apply equally to the working fluid and lubricant (if required) or any practical combinations of both.

II. REQUIREMENTS

- A. Vehicle Design Goals. The "Vehicle Design-Goals-Six Passenger Automobile," Appendix A, shall set the configuration and performance requirements for the systems analysis. The vehicle design goals are based on equality with the composite performance of the largest selling size classification of the U.S. Automobiles (based on 1969-1970 data) with standard engine (small V-8).
- B. Low Temperature. The freezing point will be at or below -40°F unless it can be shown that freeze damage to the system will not occur and that system start-up characteristics will comply with desired vehicle design goals.
- C. Materials Compatibility. The working fluid will be compatible with all common materials used in power plant construction whether occurring singly or in groups of materials. This include common derivatives of the working fluids and materials under all system operating conditions, including minor system contamination conditions. The addition of a working fluid inhibiting or stabilizing agent is acceptable.

- D. System Constraints. The system efficiency will be the maximum attainable with each candidate fluid when utilized in that class of Rankine cycle engine for which it was established. The system efficiency will be evaluated at a sufficient number of points through the system power range to at least establish a "road load" efficiency curve. A fluid which exhibits a severely decreasing road load efficiency curve at low power levels is highly undesirable.
1. It is desired that working fluid candidates display Carnot and Rankine ideal cycle efficiencies of at least 42 and 30 percent, respectfully. This represents between a 25 and 30 percent increase in state-of-the-art performance based on desired condensing temperatures between 220°F and 250°F.
 2. A highly desirable characteristic of the working fluid is an isentropic saturated vapor line. This property would remove the necessity for having a desuperheater/regenerator in the system, thereby reducing system component cost and volume. Other fluid characteristics such as viscosity, thermal conductivity, density, specific heat, etc. which influence system volume and parasitic losses will be such as to optimize the system performance relative to volume.

- E. Safety. The working fluid and its derivatives will present a negligible health hazard in any physical state when exposed to any ambient or system conditions. The working fluid and its derivatives will not be capable of sustaining combustion under atmospheric conditions or in a high temperature environment once the auxiliary source of combustion has been removed. Explosion hazards from working fluid vapors/air mixtures shall be minimized and a test used to demonstrate this.

In the event that the Rankine cycle receives widespread acceptance as an automotive power plant it is necessary that the working fluid/lubricant when released to the environment from discarded vehicles degrade to harmless components or be itself harmless to the environment.

- F. System Fluids Cost. (Over 5 years) The total working fluid and lubricant cost (initial fill and changes if required) will not exceed \$100 per vehicle (vehicle owner cost) based on one million vehicles per year. Present oil and filter change costs approximate this figure over five years, the approximate upper limit of vehicle retention by the first owner.

- G. Stability. Working fluid/lubricant degradation within the system which does not significantly impair the power plant performance or durability is acceptable. Complex or costly hardware design to offset working fluid/lubricant inadequacies is unacceptable. Tradeoff may be established between system performance, fluid degradation and fluid replacement cost if sufficient justification is demonstrated.

III. PROGRAM TASKS

- A. The technical effort of the contract will include the following tasks:

1. Establish Working Fluid Selection Criteria - Subject to approval of the Project Officer, the contractor shall establish the selection criteria required to screen candidate working fluids and lubricants. The selection criteria will include, but not be limited to, all considerations under section "H. Requirements."
2. Provide Systems Analysis - A comprehensive steady state automotive Rankine cycle systems analysis shall be provided to evaluate system performance and operating characteristics for each candidate working fluid. The analytical models will be developed with the cognizance of the AAPS Program personnel and the system contractors for the following systems:
 - (a) Reciprocating Expander
 - (b) Rotary Expander
 - (c) Or alternate consultant if either or both of the above are unable to perform this function.

The system weight, volume, cost, net efficiency, performance, and general operating characteristics will be determined. The system models must provide expedient, efficient, and realistic results.

3. Search for Existing Fluids - A survey and an analytical search as necessary using property prediction techniques shall be conducted to determine if any existing materials are suitable for use as working fluids or lubricants in automotive Rankine cycle power systems. The search will be performed within the selection criteria established and evaluated in the systems analysis.
4. Recommendations and Conclusions - If it becomes obvious at the conclusion of task 3 that no existing fluids can meet the requirements, the contractor shall recommend a change in contract scope to provide for synthesis of new fluids based on conclusions arrived at earlier in the project.

5. Property Predication Verification - If it is determined that existing fluids promise to satisfy all requirements, properties of candidate fluids found by the survey and search technique will be determined to validate the analytical predictions. The actual properties determined shall be used in final system performance predictions.

Property tests shall include, but not necessarily be limited to, thermodynamic and transport properties, range level - toxicity data with liquid, vapor and products of combustion, thermal stability, flammability, melting point and materials compatibility.

6. Dynamic Loop Tests - As part of the final fluid evaluation procedure, the working fluid shall be circulated in a dynamic loop with temperature and pressures simulating those of the actual system as nearly as possible. Materials of construction shall be utilized typifying those of the system for which the fluid is intended. The fluids shall be circulated in the loop for a period of at least 1,000 hours and samples taken periodically to determine if there is any thermal degradation or reaction with the materials.
7. Develop Preliminary Cost Estimates - Preliminary cost estimates shall be performed for the working fluid(s) and lubricant(s) that are considered acceptable candidates and where there is evidence that they will not satisfy Item II F of the specification requirements. Where firm cost data are not available, the studies shall define a range within which the costs can reasonably be expected to fall. The lower limit of the cost range shall be based on the most optimistic conditions within practical limits. Automobile production quantities of 5 million per year shall be considered for the cost estimates.

- B. Computer Programs. All computer programs developed during this project will be made available to the Government including the following support material:

- (1) A listing of all nomenclature used.
- (2) A listing of input data required to run the program.
- (3) A description and explanation of the computer output.
- (4) Running instructions.

APPENDIX B

THERMODYNAMIC PROPERTIES OF FINAL CANDIDATE RC-1

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO E1393 P 1
9/ 6/72

COMPOSITION	MOLE %	MASS %	MOLE WT
1 PFSH	60.000	57.536	168.07
2 HFA	40.000	42.463	186.06
MIXTURE	100.000	100.000	175.26

THERMODYNAMIC PROPERTIES AT SATURATION

TEMP	BUBBLE POINT LIQUID			
T	P	D	H	S
DEG F	PSI	LB/FT3	BTU/LB	HTU/LB-F
180.00	14.39	82.16	37.23	0.7112E-01
200.00	20.00	79.14	42.83	0.7986E-01
220.00	27.31	76.07	48.58	0.8846E-01
240.00	36.66	72.96	54.47	0.9695E-01
260.00	48.48	69.79	60.51	0.1053
280.00	63.20	66.55	66.71	0.1137
300.00	81.32	63.21	73.09	0.1220
320.00	103.39	59.77	79.65	0.1302
340.00	129.94	56.18	86.44	0.1386
360.00	161.66	52.41	93.51	0.1470
380.00	199.17	48.39	100.9	0.1556
400.00	243.21	44.01	108.9	0.1647
420.00	294.72	39.01	117.8	0.1745
440.00	356.92	32.50	128.8	0.1862

TEMP	DEW POINT GAS			
T	P	D	H	S
DEG F	PSI	LB/FT3	BTU/LB	HTU/LB-F
180.00	14.31	0.3781	116.4	0.2026
200.00	19.91	0.5151	119.8	0.2042
220.00	27.19	0.6914	123.2	0.2059
240.00	36.52	0.9158	126.6	0.2076
260.00	48.31	1.199	130.0	0.2095
280.00	63.01	1.555	133.3	0.2114
300.00	81.10	2.001	136.7	0.2133
320.00	103.14	2.558	140.0	0.2152
340.00	129.69	3.257	143.1	0.2171
360.00	161.38	4.141	146.2	0.2189
380.00	198.88	5.277	149.0	0.2205
400.00	242.93	6.781	151.5	0.2219
420.00	294.46	8.899	153.5	0.2227
440.00	356.73	12.64	153.8	0.2219

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 2
 9/ 6/72

COMPOSITION	MOLE %	MASS %	MOLE WT
1 C ₆ F ₅ H	40.000	57.536	168.07
2 C ₆ F ₆	40.000	42.463	186.06
MIXTURE	100.000	100.000	175.26

THERMODYNAMIC PROPERTIES IN SINGLE PHASE REGION

TEMP	D	D	H	S
T DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
180.00	10.00	0.2614	116.7	0.2069
200.00	10.00	0.2530	120.2	0.2124
220.00	10.00	0.2451	123.9	0.2179
240.00	10.00	0.2377	127.7	0.2234
260.00	10.00	0.2308	131.5	0.2288
280.00	10.00	0.2243	135.5	0.2341
300.00	10.00	0.2181	139.5	0.2395
320.00	10.00	0.2123	143.5	0.2448
340.00	10.00	0.2068	147.7	0.2500
360.00	10.00	0.2016	151.9	0.2552
380.00	10.00	0.1966	156.2	0.2604
400.00	10.00	0.1919	160.6	0.2656
420.00	10.00	0.1874	165.0	0.2707
440.00	10.00	0.1832	169.5	0.2757
460.00	10.00	0.1791	174.1	0.2807
480.00	10.00	0.1752	178.7	0.2857
500.00	10.00	0.1714	183.4	0.2907
520.00	10.00	0.1679	188.2	0.2956
540.00	10.00	0.1644	193.0	0.3005
560.00	10.00	0.1612	197.9	0.3053
580.00	10.00	0.1580	202.8	0.3101
600.00	10.00	0.1550	207.8	0.3149
620.00	10.00	0.1521	212.9	0.3196
640.00	10.00	0.1492	218.0	0.3243
660.00	10.00	0.1465	223.2	0.3289
680.00	10.00	0.1439	228.4	0.3336
700.00	10.00	0.1414	233.6	0.3381
720.00	10.00	0.1390	239.0	0.3427
740.00	10.00	0.1366	244.4	0.3472
760.00	10.00	0.1344	249.8	0.3517
780.00	10.00	0.1322	255.2	0.3562
800.00	10.00	0.1301	260.8	0.3606
180.00	14.70	82.16	37.23	0.7112E-01
200.00	14.70	0.3757	120.0	0.2078
220.00	14.70	0.3637	123.7	0.2133

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

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TEMP T DEG F	D PSI	D LB/FT3	H BTU/LB	S BTU/LB-F
240.00	14.70	0.3525	127.5	0.2189
260.00	14.70	0.3420	131.4	0.2242
280.00	14.70	0.3321	135.3	0.2296
300.00	14.70	0.3228	139.3	0.2350
320.00	14.70	0.3141	143.4	0.2403
340.00	14.70	0.3058	147.5	0.2455
360.00	14.70	0.2979	151.8	0.2508
380.00	14.70	0.2905	156.1	0.2559
400.00	14.70	0.2834	160.4	0.2611
420.00	14.70	0.2767	164.9	0.2662
440.00	14.70	0.2703	169.4	0.2713
460.00	14.70	0.2642	173.9	0.2763
480.00	14.70	0.2584	178.6	0.2813
500.00	14.70	0.2528	183.3	0.2862
520.00	14.70	0.2475	188.0	0.2911
540.00	14.70	0.2424	192.9	0.2960
560.00	14.70	0.2375	197.8	0.3009
580.00	14.70	0.2328	202.7	0.3057
600.00	14.70	0.2283	207.7	0.3104
620.00	14.70	0.2240	212.8	0.3152
640.00	14.70	0.2198	217.9	0.3199
660.00	14.70	0.2158	223.1	0.3245
680.00	14.70	0.2120	228.3	0.3291
700.00	14.70	0.2082	233.6	0.3337
720.00	14.70	0.2046	238.9	0.3383
740.00	14.70	0.2012	244.3	0.3429
760.00	14.70	0.1978	249.7	0.3473
780.00	14.70	0.1946	255.2	0.3518
800.00	14.70	0.1914	260.7	0.3562
180.00	25.00	82.16	37.22	0.7104E-01
200.00	25.00	79.14	42.83	0.7984E-01
220.00	25.00	0.6327	123.3	0.2069
240.00	25.00	0.6120	127.1	0.2124
260.00	25.00	0.5927	130.9	0.2179
280.00	25.00	0.5748	134.9	0.2233
300.00	25.00	0.5579	138.9	0.2286
320.00	25.00	0.5421	143.0	0.2340
340.00	25.00	0.5273	147.2	0.2392
360.00	25.00	0.5132	151.4	0.2445
380.00	25.00	0.5000	155.7	0.2497

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

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TEMP T DEG F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-F
400.00	25.00	0.4874	160.1	0.2600
420.00	25.00	0.4755	164.6	0.2650
440.00	25.00	0.4642	169.1	0.2701
460.00	25.00	0.4535	173.7	0.2751
480.00	25.00	0.4433	178.3	0.2800
500.00	25.00	0.4335	183.0	0.2850
520.00	25.00	0.4242	187.8	0.2898
540.00	25.00	0.4152	192.6	0.2947
560.00	25.00	0.4067	197.5	0.2995
580.00	25.00	0.3985	202.5	0.3043
600.00	25.00	0.3907	207.5	0.3090
620.00	25.00	0.3831	212.6	0.3137
640.00	25.00	0.3759	217.7	0.3184
660.00	25.00	0.3689	222.9	0.3230
680.00	25.00	0.3622	228.1	0.3276
700.00	25.00	0.3558	233.4	0.3322
720.00	25.00	0.3496	238.7	0.3367
740.00	25.00	0.3435	244.1	0.3412
760.00	25.00	0.3378	249.5	0.3456
780.00	25.00	0.3321	255.0	0.3501
800.00	25.00	0.3267	260.5	0.7097E-01
140.00	50.00	82.16	37.21	0.7972E-01
200.00	50.00	79.14	42.82	0.8835E-01
220.00	50.00	76.07	48.56	0.9688E-01
240.00	50.00	72.96	54.46	0.1053
260.00	50.00	69.79	60.51	0.2145
280.00	50.00	1.203	133.9	0.2200
300.00	50.00	1.163	138.0	0.2253
320.00	50.00	1.126	142.1	0.2307
340.00	50.00	1.092	146.3	0.2360
360.00	50.00	1.060	150.6	0.2412
380.00	50.00	1.030	155.0	0.2464
400.00	50.00	1.002	159.4	0.2516
420.00	50.00	0.9759	163.9	0.2567
440.00	50.00	0.9510	168.4	0.2617
460.00	50.00	0.9275	173.0	0.2664
480.00	50.00	0.9052	177.7	0.2717
500.00	50.00	0.8841	182.4	0.2767
520.00	50.00	0.8640	187.2	0.2816
540.00	50.00	0.8449	192.1	

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

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 9/ 6/72

TEMP T °F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-°F
560.00	50.00	0.8266	197.0	0.2865
580.00	50.00	0.8042	202.0	0.2913
600.00	50.00	0.7926	207.0	0.2961
620.00	50.00	0.7766	212.1	0.3008
640.00	50.00	0.7614	217.2	0.3056
660.00	50.00	0.7467	222.4	0.3102
680.00	50.00	0.7327	227.7	0.3149
700.00	50.00	0.7192	233.0	0.3195
720.00	50.00	0.7062	238.3	0.3241
740.00	50.00	0.6937	243.7	0.3286
760.00	50.00	0.6816	249.1	0.3331
780.00	50.00	0.6700	254.6	0.3376
800.00	50.00	0.6588	260.2	0.3420
100.00	100.00	82.16	37.19	0.7077E-01
200.00	100.00	79.14	42.78	0.7957E-01
220.00	100.00	76.07	48.52	0.8810E-01
240.00	100.00	72.96	54.39	0.9661E-01
260.00	100.00	69.79	60.43	0.1050
280.00	100.00	66.55	66.63	0.1134
300.00	100.00	63.21	73.03	0.1218
320.00	100.00	2.464	140.1	0.2157
340.00	100.00	2.369	144.4	0.2212
360.00	100.00	2.283	148.8	0.2266
380.00	100.00	2.204	153.3	0.2320
400.00	100.00	2.132	157.8	0.2373
420.00	100.00	2.066	162.3	0.2425
440.00	100.00	2.004	166.9	0.2477
460.00	100.00	1.947	171.6	0.2529
480.00	100.00	1.894	176.4	0.2579
500.00	100.00	1.844	181.1	0.2630
520.00	100.00	1.796	186.0	0.2680
540.00	100.00	1.752	190.9	0.2729
560.00	100.00	1.710	195.9	0.2779
580.00	100.00	1.671	200.9	0.2827
600.00	100.00	1.633	205.9	0.2876
620.00	100.00	1.597	211.1	0.2923
640.00	100.00	1.563	216.2	0.2971
660.00	100.00	1.531	221.5	0.3018
680.00	100.00	1.500	226.7	0.3065
700.00	100.00	1.470	232.1	0.3111

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 6
 9/ 6/72

TEMP T DEG F	P PSI	D LB/FT3	H BTU/LB	S BTU/LB-F
720.00	100.00	1.442	237.4	0.3157
740.00	100.00	1.415	242.9	0.3203
760.00	100.00	1.388	248.3	0.3248
780.00	100.00	1.363	253.9	0.3293
800.00	100.00	1.339	259.4	0.3337
180.00	300.00	82.16	37.12	0.6994E-01
200.00	300.00	79.14	42.66	0.7860E-01
220.00	300.00	76.07	48.33	0.8712E-01
240.00	300.00	72.96	54.14	0.9551E-01
260.00	300.00	69.79	60.08	0.1038
280.00	300.00	66.55	66.17	0.1121
300.00	300.00	63.21	72.42	0.1203
320.00	300.00	59.77	78.87	0.1285
340.00	300.00	56.18	85.54	0.1367
360.00	300.00	52.41	92.52	0.1452
380.00	300.00	48.39	99.93	0.1540
400.00	300.00	44.01	108.1	0.1634
420.00	300.00	39.01	117.7	0.1743
440.00	300.00	33.96	158.7	0.2285
460.00	300.00	7.782	164.2	0.2345
480.00	300.00	7.304	169.5	0.2402
500.00	300.00	6.914	174.8	0.2458
520.00	300.00	6.585	180.1	0.2512
540.00	300.00	6.300	185.3	0.2565
560.00	300.00	6.049	190.6	0.2617
580.00	300.00	5.826	195.9	0.2669
600.00	300.00	5.625	201.2	0.2719
620.00	300.00	5.442	206.5	0.2769
640.00	300.00	5.275	211.9	0.2819
660.00	300.00	5.122	217.3	0.2867
680.00	300.00	4.979	222.8	0.2916
700.00	300.00	4.847	228.3	0.2963
720.00	300.00	4.724	233.8	0.3011
740.00	300.00	4.608	239.3	0.3057
760.00	300.00	4.499	244.9	0.3104
780.00	300.00	4.397	250.6	0.3149
800.00	300.00	4.300	256.3	0.3195
180.00	700.00	82.16	36.96	0.6829E-01
200.00	700.00	79.14	42.41	0.7680E-01
220.00	700.00	76.07	47.96	0.8514E-01

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 7
9/ 6/72

TEMP T DEG F	P PSI	V LB/FT3	H BTU/LB	S BTU/LB-F
240.00	700.00	72.96	53.62	0.9333E-01
260.00	700.00	69.79	59.39	0.1014
280.00	700.00	66.55	65.25	0.1093
300.00	700.00	63.21	71.21	0.1171
320.00	700.00	59.77	77.27	0.1248
340.00	700.00	56.18	83.41	0.1324
360.00	700.00	52.41	89.64	0.1400
380.00	700.00	48.39	95.92	0.1474
400.00	700.00	44.01	102.1	0.1546
420.00	700.00	39.01	107.9	0.1610
440.00	700.00	32.50	107.5	0.1604
460.00	700.00	36.65	139.5	0.2037
480.00	700.00	36.05	144.6	0.2092
500.00	700.00	33.21	151.5	0.2165
520.00	700.00	30.11	158.7	0.2230
540.00	700.00	26.90	166.1	0.2314
560.00	700.00	23.88	173.6	0.2388
580.00	700.00	21.34	180.8	0.2459
600.00	700.00	19.35	187.8	0.2525
620.00	700.00	17.79	194.4	0.2587
640.00	700.00	16.55	200.8	0.2646
660.00	700.00	15.54	207.1	0.2702
680.00	700.00	14.70	213.3	0.2757
700.00	700.00	13.97	219.3	0.2810
720.00	700.00	13.35	225.4	0.2862
740.00	700.00	12.80	231.4	0.2912
760.00	700.00	12.32	237.4	0.2962
780.00	700.00	11.88	243.4	0.3011
800.00	700.00	11.48	249.5	0.3059
140.00	900.00	82.16	36.89	0.6747E-01
200.00	900.00	79.14	42.28	0.7590E-01
220.00	900.00	76.07	47.78	0.8415E-01
240.00	900.00	72.96	53.37	0.9224E-01
260.00	900.00	69.79	59.04	0.1002
280.00	900.00	66.55	64.79	0.1070
300.00	900.00	63.21	70.61	0.1155
320.00	900.00	59.77	76.47	0.1230
340.00	900.00	56.18	82.35	0.1303
360.00	900.00	52.41	88.20	0.1373
380.00	900.00	48.39	93.91	0.1441

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 8
9/ 6/72

TEMP T DEG F	P PSI	D LB/FT3	H BTU/LB	S BTU/LB-F
400.00	900.00	44.01	99.18	0.1501
420.00	900.00	39.01	102.9	0.1544
440.00	900.00	32.50	95.11	0.1454
460.00	900.00	41.83	136.7	0.1997
480.00	900.00	39.87	142.8	0.2063
500.00	900.00	37.83	149.0	0.2129
520.00	900.00	35.70	155.4	0.2195
540.00	900.00	33.51	162.0	0.2261
560.00	900.00	31.29	168.6	0.2327
580.00	900.00	29.10	175.3	0.2392
600.00	900.00	27.01	182.1	0.2456
620.00	900.00	25.10	188.8	0.2519
640.00	900.00	23.39	195.5	0.2580
660.00	900.00	21.89	202.0	0.2639
680.00	900.00	20.59	208.5	0.2697
700.00	900.00	19.46	214.9	0.2752
720.00	900.00	18.45	221.2	0.2806
740.00	900.00	17.61	227.5	0.2859
760.00	900.00	16.85	233.7	0.2910
780.00	900.00	16.17	239.9	0.2961
800.00	900.00	15.56	246.1	0.3010
100.00	1000.00	82.16	36.85	0.6706E-01
200.00	1000.00	79.14	42.22	0.7545E-01
220.00	1000.00	76.07	47.69	0.8366E-01
240.00	1000.00	72.96	53.24	0.9169E-01
260.00	1000.00	69.79	58.87	0.9955E-01
280.00	1000.00	66.55	64.56	0.1072
300.00	1000.00	63.21	70.30	0.1148
320.00	1000.00	59.77	76.07	0.1221
340.00	1000.00	56.18	81.82	0.1292
360.00	1000.00	52.41	87.48	0.1360
380.00	1000.00	48.39	92.90	0.1424
400.00	1000.00	44.01	97.69	0.1479
420.00	1000.00	39.01	100.5	0.1510
440.00	1000.00	32.50	88.92	0.1379
460.00	1000.00	43.05	136.2	0.1988
480.00	1000.00	41.27	142.2	0.2052
500.00	1000.00	39.43	148.4	0.2117
520.00	1000.00	37.54	154.6	0.2181
540.00	1000.00	35.60	160.9	0.2245

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 9
9/ 6/72

TEMP T DEG F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-F
560.00	1000.00	33.63	167.3	0.2304
580.00	1000.00	31.68	173.8	0.2371
600.00	1000.00	29.77	180.4	0.2434
620.00	1000.00	27.95	187.0	0.2495
640.00	1000.00	26.26	193.5	0.2556
660.00	1000.00	24.71	200.1	0.2615
680.00	1000.00	23.32	206.6	0.2672
700.00	1000.00	22.07	213.0	0.2729
720.00	1000.00	20.97	219.4	0.2783
740.00	1000.00	19.98	225.7	0.2836
760.00	1000.00	19.10	232.0	0.2889
780.00	1000.00	18.32	238.3	0.2939
800.00	1000.00	17.61	244.6	0.2989
180.00	1050.00	82.16	36.83	0.6685E-01
200.00	1050.00	79.14	42.19	0.7523E-01
220.00	1050.00	76.07	47.64	0.8341E-01
240.00	1050.00	72.96	53.17	0.9142E-01
260.00	1050.00	69.79	58.78	0.9925E-01
280.00	1050.00	66.55	64.45	0.1069
300.00	1050.00	63.21	70.15	0.1144
320.00	1050.00	59.77	75.87	0.1216
340.00	1050.00	56.18	81.56	0.1287
360.00	1050.00	52.41	87.12	0.1354
380.00	1050.00	48.39	92.40	0.1416
400.00	1050.00	44.01	96.95	0.1468
420.00	1050.00	39.01	99.26	0.1494
440.00	1050.00	32.50	85.82	0.1341
460.00	1050.00	43.60	136.1	0.1983
480.00	1050.00	41.89	142.0	0.2047
500.00	1050.00	40.13	148.1	0.2111
520.00	1050.00	38.33	154.2	0.2175
540.00	1050.00	36.49	160.5	0.2239
560.00	1050.00	34.62	166.8	0.2301
580.00	1050.00	32.77	173.2	0.2363
600.00	1050.00	30.94	179.7	0.2425
620.00	1050.00	29.18	186.2	0.2486
640.00	1050.00	27.52	192.7	0.2545
660.00	1050.00	25.98	199.2	0.2604
680.00	1050.00	24.57	205.7	0.2661
700.00	1050.00	23.30	212.2	0.2717

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 10
 9/ 6/72

TEMP T DEG F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-F
720.00	1050.00	22.15	218.6	0.2772
740.00	1050.00	21.12	224.9	0.2826
760.00	1050.00	20.20	231.3	0.2878
780.00	1050.00	19.37	237.6	0.2929
800.00	1050.00	18.62	243.9	0.2980
100.00	1150.00	82.16	36.79	0.6644E-01
200.00	1150.00	79.14	42.13	0.7478E-01
220.00	1150.00	76.07	47.55	0.8292E-01
240.00	1150.00	72.96	53.05	0.9087E-01
260.00	1150.00	69.79	58.61	0.9864E-01
280.00	1150.00	66.55	64.22	0.1062
300.00	1150.00	63.21	69.85	0.1136
320.00	1150.00	59.77	75.47	0.1207
340.00	1150.00	56.18	81.02	0.1276
360.00	1150.00	52.41	86.41	0.1341
380.00	1150.00	48.39	91.40	0.1399
400.00	1150.00	44.01	95.47	0.1446
420.00	1150.00	39.01	96.81	0.1460
440.00	1150.00	32.50	79.62	0.1266
460.00	1150.00	44.60	135.8	0.1976
480.00	1150.00	43.02	141.7	0.2039
500.00	1150.00	41.39	147.6	0.2102
520.00	1150.00	39.73	153.7	0.2164
540.00	1150.00	38.05	159.8	0.2226
560.00	1150.00	36.35	166.0	0.2288
580.00	1150.00	34.65	172.3	0.2349
600.00	1150.00	32.97	178.6	0.2409
620.00	1150.00	31.33	185.0	0.2469
640.00	1150.00	29.75	191.4	0.2528
660.00	1150.00	28.26	197.9	0.2586
680.00	1150.00	26.86	204.3	0.2642
700.00	1150.00	25.57	210.7	0.2698
720.00	1150.00	24.38	217.1	0.2753
740.00	1150.00	23.29	223.5	0.2807
760.00	1150.00	22.30	229.9	0.2859
780.00	1150.00	21.40	236.2	0.2911
800.00	1150.00	20.52	242.6	0.2962
100.00	1300.00	82.16	36.73	0.6582E-01
200.00	1300.00	79.14	42.03	0.7410E-01
220.00	1300.00	76.07	47.41	0.8218E-01

THEMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 11
9/ 6/72

TEMP T DEG F	P PSI	D LR/FT3	H BTU/LB	S BTU/LB-F
240.00	1300.00	72.96	52.85	0.9005E-01
260.00	1300.00	69.79	58.35	0.9772E-01
280.00	1300.00	66.55	63.87	0.1052
300.00	1300.00	63.21	69.40	0.1124
320.00	1300.00	59.77	74.87	0.1194
340.00	1300.00	56.18	80.23	0.1260
360.00	1300.00	52.41	85.33	0.1321
380.00	1300.00	48.39	89.89	0.1375
400.00	1300.00	44.01	93.24	0.1413
420.00	1300.00	39.01	93.12	0.1410
440.00	1300.00	32.50	70.33	0.1153
460.00	1300.00	45.92	135.5	0.1966
480.00	1300.00	44.47	141.2	0.2028
500.00	1300.00	43.00	147.1	0.2090
520.00	1300.00	41.51	153.0	0.2151
540.00	1300.00	40.00	159.0	0.2211
560.00	1300.00	38.47	165.1	0.2272
580.00	1300.00	36.95	171.3	0.2331
600.00	1300.00	35.45	177.5	0.2390
620.00	1300.00	33.96	183.7	0.2449
640.00	1300.00	32.51	190.0	0.2506
660.00	1300.00	31.11	196.3	0.2563
680.00	1300.00	29.78	202.7	0.2619
700.00	1300.00	28.51	209.0	0.2675
720.00	1300.00	27.32	215.4	0.2729
740.00	1300.00	26.20	221.7	0.2783
760.00	1300.00	25.17	228.1	0.2835
780.00	1300.00	24.20	234.4	0.2887
800.00	1300.00	23.31	240.8	0.2938
1200.00	1500.00	82.16	36.66	0.6499E-01
200.00	1500.00	79.14	41.91	0.7320E-01
220.00	1500.00	76.07	47.22	0.8119E-01
240.00	1500.00	72.96	52.60	0.8894E-01
260.00	1500.00	69.79	58.00	0.9651E-01
280.00	1500.00	66.55	63.41	0.1038
300.00	1500.00	63.21	68.79	0.1108
320.00	1500.00	59.77	74.07	0.1175
340.00	1500.00	56.18	79.17	0.1238
360.00	1500.00	52.41	83.89	0.1295
380.00	1500.00	48.39	87.88	0.1341

THE THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 12
9/ 6/72

TEMP T DEG F	D PSI	D LB/FT3	H BTU/LB	S BTU/LB-F
400.00	1500.00	44.01	90.28	0.1364
420.00	1500.00	39.01	88.21	0.1344
440.00	1500.00	32.50	57.94	0.1003
460.00	1500.00	47.42	135.2	0.1954
480.00	1500.00	46.11	140.9	0.2015
500.00	1500.00	44.79	146.7	0.2076
520.00	1500.00	43.45	152.5	0.2136
540.00	1500.00	42.10	158.4	0.2196
560.00	1500.00	40.75	164.3	0.2255
580.00	1500.00	39.40	170.3	0.2313
600.00	1500.00	38.06	176.4	0.2371
620.00	1500.00	36.73	182.5	0.2428
640.00	1500.00	35.42	188.7	0.2485
660.00	1500.00	34.15	194.9	0.2541
680.00	1500.00	32.91	201.1	0.2596
700.00	1500.00	31.72	207.4	0.2650
720.00	1500.00	30.57	213.7	0.2704
740.00	1500.00	29.48	220.0	0.2757
760.00	1500.00	28.45	226.3	0.2809
780.00	1500.00	27.47	232.6	0.2861
800.00	1500.00	26.55	239.0	0.2911

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
PENTAFLUOROBENZENE, HEXAFLUOROBENZENE 60/40 MOLE RATIO

E1393 P 13
9/ 6/72

THERMODYNAMIC PROPERTIES AT SATURATION

BUBBLE POINT LIQUID - - - - -				
TEMP T	P	D	H	S
DEG F	PSI	LB/FT3	BTU/LB	BTU/LB-F
159.17	10.00	85.27	31.53	0.6186E-01
181.25	14.70	81.97	37.57	0.7167E-01
214.22	25.00	76.96	46.91	0.8599E-01
262.24	50.00	69.42	61.21	0.1063
317.17	100.00	60.26	78.71	0.1291
421.88	300.00	38.49	118.7	0.1755

DEW POINT GAS - - - - -				
TEMP T	P	D	H	S
DEG F	PSI	LB/FT3	BTU/LB	BTU/LB-F
159.5	10.00	0.2707	113.1	0.2011
181.54	14.70	0.3876	116.7	0.2027
214.51	25.00	0.6386	122.3	0.2054
262.53	50.00	1.240	130.4	0.2097
317.37	100.00	2.477	139.5	0.2150
421.97	300.00	9.161	153.6	0.2227

APPENDIX C

THERMODYNAMIC PROPERTIES OF FINAL CANDIDATE RC-2

THE THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYLPYRIDINE, WATER 35 MOLE PC ORGANIC

E1393 P 1
9/ 1/72

COMPOSITION	MOLE %	MASS %	MOLE WT
1 2ME PYRIDINE	35.000	73.549	93.13
2 WATER	65.000	26.431	18.02
TOTAL	100.000	100.000	44.31

THE THERMODYNAMIC PROPERTIES AT SATURATION

T, °F	D	H	M	S
DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
140.00	10.69	54.85	104.7	0.1403
200.00	15.85	56.26	125.9	0.2023
220.00	22.04	56.62	142.4	0.2277
240.00	32.44	54.97	159.3	0.2465
260.00	44.07	54.18	176.6	0.2624
280.00	61.05	53.37	194.3	0.2754
300.00	81.51	52.40	212.4	0.2854
320.00	107.18	51.52	230.9	0.2939
340.00	138.89	50.48	250.0	0.3061
360.00	177.69	49.33	269.6	0.3171
380.00	224.82	48.08	289.8	0.3274
400.00	282.30	46.70	310.6	0.3372
420.00	352.34	45.18	332.4	0.3462
440.00	436.74	43.51	355.1	0.3544
460.00	539.01	41.05	379.0	0.3615
480.00	664.54	39.58	404.5	0.3676
500.00	823.00	37.25	432.4	0.3727
520.00	1031.02	34.62	463.6	0.3768
540.00	1292.14	31.62	500.6	0.3800
560.00	1516.55	28.15	544.4	0.3823

T, °F	D	H	M	S
DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
140.00	8.77	0.6215-01	490.6	0.3773
200.00	12.20	0.7725-01	497.5	0.3808
220.00	17.46	0.1077	504.4	0.3833
240.00	24.46	0.1473	511.3	0.3855
260.00	33.67	0.1940	518.2	0.3873
280.00	45.44	0.2421	525.2	0.3887
300.00	60.44	0.3023	532.1	0.3898
320.00	74.37	0.4420	539.0	0.3904
340.00	102.82	0.5650	545.7	0.3906
360.00	131.84	0.7165	552.4	0.3903

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 2-METHYLPYRROLIDINE, WATER 35 MOLE PC ORGANIC

1393 P 2
 9/ 1/77

TEMP	- - - - - DEW POINT GAS - - - - -			
T	P	n	H	S
DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
320.00	167.52	0.9033	558.4	0.8002
400.00	211.30	1.135	565.1	0.7991
420.00	266.00	1.430	570.8	0.7956
440.00	339.60	1.846	575.7	0.7916
460.00	437.54	2.430	579.1	0.7881
480.00	569.18	3.334	580.3	0.7741
500.00	752.64	4.408	576.3	0.7600
520.00	1006.84	10.00	546.7	0.7272
540.00	1290.71	13.38	538.4	0.7168
560.00	1512.92	16.12	533.0	0.7072

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYLPYRIDINE, WATER 35 MOLE PC ORGANIC

E1393 P 3
9/ 1/72

COMPOSITION	MOLE %	MASS %	MOLE WT
1 2ME PYRIDINE	35.000	73.569	93.13
2 WATER	65.000	26.431	18.02
MIXTURE	100.000	100.000	44.31

THERMODYNAMIC PROPERTIES IN SINGLE PHASE REGION

T, MP	P	D	H	S
DEG F	PSI	LB/FT3	BTU/LB	BTU/LB-F
120.00	5.00	0.3244E-01	490.4	0.8604
200.00	5.00	0.3144E-01	498.0	0.8714
220.00	5.00	0.3050E-01	505.3	0.8822
240.00	5.00	0.2962E-01	512.6	0.8929
260.00	5.00	0.2879E-01	520.1	0.9035
280.00	5.00	0.2800E-01	527.8	0.9130
300.00	5.00	0.2726E-01	535.5	0.9243
320.00	5.00	0.2656E-01	543.4	0.9342
340.00	5.00	0.2589E-01	551.4	0.9447
360.00	5.00	0.2525E-01	559.6	0.9547
380.00	5.00	0.2464E-01	567.8	0.9647
400.00	5.00	0.2407E-01	576.2	0.9745
420.00	5.00	0.2352E-01	584.7	0.9843
440.00	5.00	0.2299E-01	593.3	0.9940
460.00	5.00	0.2249E-01	602.0	1.004
480.00	5.00	0.2201E-01	610.9	1.013
500.00	5.00	0.2155E-01	619.8	1.022
520.00	5.00	0.2110E-01	628.9	1.032
540.00	5.00	0.2068E-01	638.0	1.041
560.00	5.00	0.2027E-01	647.3	1.050
580.00	5.00	0.1988E-01	656.6	1.059
600.00	5.00	0.1950E-01	666.1	1.069
620.00	5.00	0.1914E-01	675.6	1.077
640.00	5.00	0.1879E-01	685.3	1.086
660.00	5.00	0.1846E-01	695.0	1.095
680.00	5.00	0.1813E-01	704.9	1.104
700.00	5.00	0.1782E-01	714.8	1.112
720.00	5.00	0.1751E-01	724.9	1.121
740.00	5.00	0.1722E-01	735.0	1.129
760.00	5.00	0.1694E-01	745.2	1.139
780.00	5.00	0.1666E-01	755.5	1.145
800.00	5.00	0.1640E-01	765.8	1.154
120.00	10.00	0.0	0.0	0.0
200.00	10.00	0.6318E-01	497.6	0.8390
220.00	10.00	0.6128E-01	504.9	0.8502

THE THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYLPYRIDINE, WATER 35 MOLE PC ORGANIC

F. 393 P. 4
9/ 1/72

T DEG F	D PSI	η LB/FT ³	H BTU/LB	S BTU/LB-F
240.00	10.00	0.5949E-01	512.3	0.8615
240.00	10.00	0.5780E-01	519.8	0.8721
240.00	10.00	0.5621E-01	527.5	0.8826
300.00	10.00	0.5470E-01	535.2	0.8929
320.00	10.00	0.5327E-01	543.1	0.9032
340.00	10.00	0.5192E-01	551.2	0.9134
340.00	10.00	0.5063E-01	559.3	0.9234
340.00	10.00	0.4941E-01	567.6	0.9334
400.00	10.00	0.4825E-01	576.0	0.9433
420.00	10.00	0.4714E-01	584.5	0.9530
440.00	10.00	0.4608E-01	593.1	0.9627
440.00	10.00	0.4504E-01	601.4	0.9724
440.00	10.00	0.4409E-01	610.7	0.9818
500.00	10.00	0.4317E-01	619.6	0.9914
520.00	10.00	0.4228E-01	628.7	1.001
540.00	10.00	0.4142E-01	637.8	1.010
540.00	10.00	0.4060E-01	647.1	1.019
540.00	10.00	0.3982E-01	656.4	1.024
600.00	10.00	0.3906E-01	665.9	1.037
620.00	10.00	0.3833E-01	675.5	1.045
640.00	10.00	0.3763E-01	685.1	1.055
640.00	10.00	0.3695E-01	694.9	1.064
640.00	10.00	0.3630E-01	704.7	1.072
700.00	10.00	0.3567E-01	714.7	1.081
720.00	10.00	0.3506E-01	724.7	1.090
740.00	10.00	0.3447E-01	734.8	1.099
740.00	10.00	0.3391E-01	745.0	1.107
740.00	10.00	0.3336E-01	755.3	1.115
800.00	10.00	0.3282E-01	765.7	1.123
140.00	14.70	56.85	109.7	0.1403
200.00	14.70	0.0	0.0	0.0
220.00	14.70	0.9044E-01	504.6	0.8332
240.00	14.70	0.8776E-01	512.0	0.8433
240.00	14.70	0.8525E-01	519.5	0.8545
240.00	14.70	0.8288E-01	527.2	0.8650
300.00	14.70	0.8064E-01	535.0	0.8754
320.00	14.70	0.7852E-01	542.9	0.8857
340.00	14.70	0.7651E-01	550.9	0.8959
340.00	14.70	0.7460E-01	559.1	0.9060
340.00	14.70	0.7278E-01	567.3	0.9160

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYLPYRIDINE, WATER 35 MOLE PC ORGANIC

E1393 P 5
9/ 1/72

TEMP T DEG F	P PSI	U LR/FT3	H BTU/LH	S BTU/LH-F
400.00	14.70	0.7106E-01	575.7	0.9252
420.00	14.70	0.6941E-01	584.2	0.9354
440.00	14.70	0.6784E-01	592.9	0.9453
460.00	14.70	0.6634E-01	601.6	0.9549
480.00	14.70	0.6491E-01	610.5	0.9644
500.00	14.70	0.6354E-01	619.4	0.9739
520.00	14.70	0.6222E-01	628.5	0.9832
540.00	14.70	0.6096E-01	637.6	0.9925
560.00	14.70	0.5975E-01	646.9	1.002
580.00	14.70	0.5859E-01	656.3	1.011
600.00	14.70	0.5747E-01	665.7	1.021
620.00	14.70	0.5640E-01	675.3	1.029
640.00	14.70	0.5536E-01	685.0	1.039
660.00	14.70	0.5436E-01	694.7	1.046
680.00	14.70	0.5340E-01	704.6	1.055
700.00	14.70	0.5247E-01	714.5	1.064
720.00	14.70	0.5157E-01	724.6	1.072
740.00	14.70	0.5071E-01	734.7	1.081
760.00	14.70	0.4987E-01	744.9	1.089
780.00	14.70	0.4906E-01	755.2	1.097
800.00	14.70	0.4827E-01	765.6	1.106
180.00	25.00	56.85	109.8	0.1802
200.00	25.00	56.26	125.9	0.2022
220.00	25.00	55.62	142.4	0.2237
240.00	25.00	0.0	0.0	0.0
260.00	25.00	0.1462	518.8	0.8301
280.00	25.00	0.1420	526.5	0.8407
300.00	25.00	0.1381	534.3	0.8511
320.00	25.00	0.1344	542.3	0.8614
340.00	25.00	0.1309	550.3	0.8716
360.00	25.00	0.1276	558.5	0.8817
380.00	25.00	0.1245	566.8	0.8917
400.00	25.00	0.1215	575.2	0.9016
420.00	25.00	0.1186	583.8	0.9114
440.00	25.00	0.1159	592.4	0.9211
460.00	25.00	0.1133	601.1	0.9308
480.00	25.00	0.1108	610.0	0.9403
500.00	25.00	0.1085	619.0	0.9497
520.00	25.00	0.1062	628.1	0.9591
540.00	25.00	0.1040	637.2	0.9686

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYLPYRIDINE. WATER 35 MOLE PC ORGANIC

E1393 P 6
9/ 1/72

T °F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-°F
560.00	25.00	0.1019	646.5	0.9774
580.00	25.00	0.9995E-01	655.9	0.9867
600.00	25.00	0.9803E-01	665.4	0.9957
620.00	25.00	0.9618E-01	675.0	1.005
640.00	25.00	0.9440E-01	684.6	1.014
660.00	25.00	0.9268E-01	694.4	1.022
680.00	25.00	0.9103E-01	704.3	1.031
700.00	25.00	0.8944E-01	714.2	1.040
720.00	25.00	0.8790E-01	724.3	1.048
740.00	25.00	0.8642E-01	734.4	1.057
760.00	25.00	0.8498E-01	744.6	1.065
780.00	25.00	0.8359E-01	754.9	1.074
800.00	25.00	0.8225E-01	765.3	1.082
140.00	50.00	56.85	109.8	0.1802
200.00	50.00	56.26	126.0	0.2022
220.00	50.00	55.62	142.5	0.2237
240.00	50.00	54.93	159.3	0.2447
260.00	50.00	54.18	176.6	0.2653
280.00	50.00	0.0	0.0	0.0
300.00	50.00	0.2810	532.8	0.8187
320.00	50.00	0.2732	540.8	0.8291
340.00	50.00	0.2652	548.9	0.8394
360.00	50.00	0.2582	557.1	0.8495
380.00	50.00	0.2521	565.5	0.8596
400.00	50.00	0.2459	574.0	0.8696
420.00	50.00	0.2399	582.5	0.8794
440.00	50.00	0.2343	591.2	0.8892
460.00	50.00	0.2289	600.0	0.8989
480.00	50.00	0.2237	608.9	0.9085
500.00	50.00	0.2182	617.9	0.9179
520.00	50.00	0.2142	627.0	0.9273
540.00	50.00	0.2097	636.3	0.9366
560.00	50.00	0.2054	645.6	0.9450
580.00	50.00	0.2013	655.0	0.9531
600.00	50.00	0.1973	664.5	0.9611
620.00	50.00	0.1935	674.1	0.9691
640.00	50.00	0.1899	683.8	0.9770
660.00	50.00	0.1864	693.6	0.9849
680.00	50.00	0.1830	703.5	0.9925
700.00	50.00	0.1798	713.5	1.0002

THERMODYNAMIC PROPERTIES OF SENIOM CANDIDATE FLUIDS
 2-METHYL PYRIDINE. WATER 35 MOLE PC ORGANIC

F1393 P 7
 9/ 1/72

TEMP T DEG F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-F
720.00	50.00	0.1766	723.5	1.017
740.00	50.00	0.1736	733.7	1.025
760.00	50.00	0.1707	743.9	1.034
780.00	50.00	0.1679	754.3	1.042
800.00	50.00	0.1651	764.7	1.051
100.00	100.00	56.85	109.9	0.1901
200.00	100.00	56.26	126.1	0.2021
220.00	100.00	55.62	142.6	0.2234
240.00	100.00	54.93	159.4	0.2446
260.00	100.00	54.18	176.7	0.2652
280.00	100.00	53.37	194.3	0.2855
300.00	100.00	52.49	212.4	0.3053
320.00	100.00	0.0	0.0	0.0
340.00	100.00	0.5485	545.9	0.4059
360.00	100.00	0.5728	554.3	0.4162
380.00	100.00	0.5181	562.4	0.4264
400.00	100.00	0.5043	571.4	0.4365
420.00	100.00	0.4912	580.0	0.4467
440.00	100.00	0.4789	588.8	0.4568
460.00	100.00	0.4672	597.7	0.4661
480.00	100.00	0.4561	606.7	0.4754
500.00	100.00	0.4456	615.4	0.4854
520.00	100.00	0.4356	625.0	0.4940
540.00	100.00	0.4260	634.3	0.5042
560.00	100.00	0.4169	643.6	0.5135
580.00	100.00	0.4082	653.1	0.5227
600.00	100.00	0.3999	662.7	0.5319
620.00	100.00	0.3919	672.4	0.5409
640.00	100.00	0.3843	682.1	0.5494
660.00	100.00	0.3770	692.0	0.5587
680.00	100.00	0.3699	701.9	0.5675
700.00	100.00	0.3632	711.9	0.5762
720.00	100.00	0.3566	722.0	0.5849
740.00	100.00	0.3504	732.2	0.5935
760.00	100.00	0.3443	742.5	1.002
780.00	100.00	0.3385	752.9	1.010
800.00	100.00	0.3328	763.3	1.019
100.00	300.00	56.85	110.4	0.1794
200.00	300.00	56.26	126.5	0.2017
220.00	300.00	55.62	143.0	0.2232

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 2-METHYLPYRIDINE, WATER 35 MOLF PC ORGANIC

E1393 P. A
 9/ 1/72

T TEMP DEG F	P PSI	D LB/FT3	H BTU/LB	S BTU/LB-F
240.00	300.00	54.93	159.8	0.2442
260.00	300.00	54.18	177.0	0.2647
280.00	300.00	53.37	194.6	0.2849
300.00	300.00	52.49	212.6	0.3047
320.00	300.00	51.52	231.1	0.3242
340.00	300.00	50.48	250.0	0.3435
360.00	300.00	49.33	269.6	0.3625
380.00	300.00	48.08	289.7	0.3814
400.00	300.00	46.70	310.6	0.4001
420.00	300.00	0.0	0.0	0.0
440.00	300.00	1.592	578.1	0.7990
460.00	300.00	1.540	587.5	0.8094
480.00	300.00	1.493	596.9	0.8195
500.00	300.00	1.449	606.5	0.8294
520.00	300.00	1.409	616.0	0.8394
540.00	300.00	1.371	625.7	0.8492
560.00	300.00	1.335	635.4	0.8598
580.00	300.00	1.302	645.2	0.8693
600.00	300.00	1.271	655.1	0.8777
620.00	300.00	1.241	665.0	0.8874
640.00	300.00	1.213	675.0	0.8962
660.00	300.00	1.186	685.1	0.9053
680.00	300.00	1.161	695.3	0.9143
700.00	300.00	1.137	705.5	0.9232
720.00	300.00	1.113	715.8	0.9321
740.00	300.00	1.091	726.2	0.9404
760.00	300.00	1.070	736.7	0.9494
780.00	300.00	1.050	747.2	0.9580
800.00	300.00	1.031	757.9	0.9665
100.00	500.00	56.85	110.8	0.1795
200.00	500.00	56.26	126.9	0.2014
220.00	500.00	55.62	143.4	0.2224
240.00	500.00	54.93	160.2	0.2437
260.00	500.00	54.18	177.3	0.2642
280.00	500.00	53.37	194.9	0.2843
300.00	500.00	52.49	212.9	0.3041
320.00	500.00	51.52	231.3	0.3235
340.00	500.00	50.48	250.1	0.3427
360.00	500.00	49.33	269.6	0.3614
380.00	500.00	48.08	289.6	0.3803

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYLPYRIDINE. WATER 35 MOLE PC ORGANIC

E1393 P 9
9/ 1/72

T-TEMP T	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-F
400.00	500.00	46.70	310.4	0.3989
420.00	500.00	45.18	332.0	0.4172
440.00	500.00	43.51	354.8	0.4344
460.00	500.00	0.0	0.0	0.0
480.00	500.00	2.784	585.1	0.7877
500.00	500.00	2.676	595.4	0.7985
520.00	500.00	2.577	605.6	0.8091
540.00	500.00	2.487	615.9	0.8194
560.00	500.00	2.405	626.1	0.8295
580.00	500.00	2.331	636.3	0.8395
600.00	500.00	2.262	646.6	0.8493
620.00	500.00	2.199	656.9	0.8589
640.00	500.00	2.139	667.3	0.8685
660.00	500.00	2.084	677.7	0.8778
680.00	500.00	2.032	688.2	0.8871
700.00	500.00	1.984	698.7	0.8962
720.00	500.00	1.938	709.3	0.9053
740.00	500.00	1.895	719.9	0.9142
760.00	500.00	1.853	730.6	0.9230
780.00	500.00	1.814	741.3	0.9318
800.00	500.00	1.777	752.1	0.9404
180.00	700.00	56.85	111.2	0.1791
200.00	700.00	56.26	127.3	0.2010
220.00	700.00	55.62	143.8	0.2224
240.00	700.00	54.93	160.5	0.2433
260.00	700.00	54.18	177.7	0.2637
280.00	700.00	53.37	195.2	0.2838
300.00	700.00	52.49	213.1	0.3035
320.00	700.00	51.52	231.4	0.3228
340.00	700.00	50.48	250.2	0.3419
360.00	700.00	49.33	269.6	0.3607
380.00	700.00	48.08	289.5	0.3793
400.00	700.00	46.70	310.1	0.3977
420.00	700.00	45.18	331.6	0.4157
440.00	700.00	43.51	354.1	0.4327
460.00	700.00	41.65	378.2	0.4488
480.00	700.00	39.58	404.3	0.4641
500.00	700.00	4.331	581.1	0.7722
520.00	700.00	4.087	592.7	0.7842
540.00	700.00	3.884	604.0	0.7956

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYLPYRIDINE, WATER 35 MOLF PC ORGANIC

F1393 P 10
9/ 1/72

TEMP T DEG F	P PSI	ρ LB/FT ³	H BTU/LB	S BTU/LB-F
560.00	700.00	3.710	615.1	0.8066
580.00	700.00	3.559	626.1	0.8174
600.00	700.00	3.425	637.0	0.8277
620.00	700.00	3.305	647.9	0.8379
640.00	700.00	3.197	658.7	0.8478
660.00	700.00	3.097	669.6	0.8574
680.00	700.00	3.006	680.4	0.8672
700.00	700.00	2.922	691.3	0.8767
720.00	700.00	2.844	702.2	0.8860
740.00	700.00	2.771	713.1	0.8952
760.00	700.00	2.703	724.1	0.9042
780.00	700.00	2.639	735.1	0.9132
800.00	700.00	2.579	746.1	0.9220
140.00	900.00	56.85	111.7	0.1783
200.00	900.00	56.26	127.6	0.2007
220.00	900.00	55.62	144.2	0.2220
240.00	900.00	54.93	160.9	0.2424
260.00	900.00	54.18	178.0	0.2632
280.00	900.00	53.37	195.5	0.2832
300.00	900.00	52.49	213.3	0.3024
320.00	900.00	51.52	231.6	0.3221
340.00	900.00	50.48	250.3	0.3411
360.00	900.00	49.33	269.6	0.3598
380.00	900.00	48.08	289.4	0.3782
400.00	900.00	46.76	309.8	0.3964
420.00	900.00	45.18	331.1	0.4147
440.00	900.00	43.51	353.4	0.4300
460.00	900.00	41.65	377.1	0.4467
480.00	900.00	39.58	402.8	0.4615
500.00	900.00	37.25	431.5	0.4730
520.00	900.00	6.477	573.3	0.7560
540.00	900.00	5.870	587.9	0.7717
560.00	900.00	5.448	601.1	0.7848
580.00	900.00	5.122	613.6	0.7960
600.00	900.00	4.856	625.6	0.8084
620.00	900.00	4.631	637.4	0.8194
640.00	900.00	4.437	649.0	0.8300
660.00	900.00	4.266	660.5	0.8404
680.00	900.00	4.114	671.9	0.8505
700.00	900.00	3.977	683.3	0.8604

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYLPYRIDINE, WATER 35 MOLE PC ORGANIC

E1393 P 11
9/ 1/72

TEMP T DEG F	P PSI	D LB/FT3	H BTU/LB	S BTU/LB-F
720.00	900.00	3.852	694.6	0.8700
740.00	900.00	3.738	705.9	0.8795
760.00	900.00	3.632	717.2	0.8884
780.00	900.00	3.535	728.5	0.8981
800.00	900.00	3.444	739.8	0.9071
180.00	1000.00	56.85	111.9	0.1787
200.00	1000.00	56.26	128.0	0.2005
220.00	1000.00	55.62	144.4	0.2214
240.00	1000.00	54.93	161.1	0.2426
260.00	1000.00	54.18	178.2	0.2630
280.00	1000.00	53.37	195.6	0.2830
300.00	1000.00	52.49	213.4	0.3024
320.00	1000.00	51.52	231.7	0.3214
340.00	1000.00	50.48	250.4	0.3407
360.00	1000.00	49.37	269.6	0.3593
380.00	1000.00	48.08	289.3	0.3777
400.00	1000.00	46.70	309.7	0.3952
420.00	1000.00	45.18	330.9	0.4132
440.00	1000.00	43.51	353.1	0.4301
460.00	1000.00	41.65	376.6	0.4457
480.00	1000.00	39.58	402.0	0.4602
500.00	1000.00	37.25	430.5	0.4723
520.00	1000.00	34.62	461.1	0.4827
540.00	1000.00	31.77	495.6	0.4915
560.00	1000.00	28.65	534.8	0.4986
580.00	1000.00	25.25	578.8	0.5043
600.00	1000.00	21.71	628.9	0.5087
620.00	1000.00	18.15	685.4	0.5118
640.00	1000.00	14.53	748.6	0.5136
660.00	1000.00	10.88	818.5	0.5143
680.00	1000.00	7.32	895.3	0.5137
700.00	1000.00	4.55	978.9	0.5119
720.00	1000.00	2.40	1069.5	0.5090
740.00	1000.00	0.26	1167.1	0.5050
760.00	1000.00	0.13	1271.6	0.5000
780.00	1000.00	0.01	1382.1	0.4941
800.00	1000.00	0.00	1500.0	0.4875
180.00	1100.00	56.85	112.1	0.1785
200.00	1100.00	56.26	128.2	0.2003
220.00	1100.00	55.62	144.5	0.2216

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 2-METHYLPYRIDINE, WATER 35 MOLE PC ORGANIC

E1393 P 12
 9/ 1/72

T DEG F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-F
240.00	1100.00	54.93	161.3	0.2424
260.00	1100.00	54.18	178.3	0.2623
280.00	1100.00	53.37	195.8	0.2827
300.00	1100.00	52.49	213.6	0.3023
320.00	1100.00	51.52	231.8	0.3214
340.00	1100.00	50.48	250.4	0.3403
360.00	1100.00	49.33	269.6	0.3589
380.00	1100.00	48.08	289.3	0.3772
400.00	1100.00	46.70	309.6	0.3952
420.00	1100.00	45.18	330.7	0.4128
440.00	1100.00	43.51	352.7	0.4292
460.00	1100.00	41.65	376.1	0.4446
480.00	1100.00	39.58	401.3	0.4589
500.00	1100.00	37.25	429.4	0.4706
520.00	1100.00	34.62	462.5	0.4627
540.00	1100.00	11.14	550.0	0.7289
560.00	1100.00	8.470	578.4	0.7571
580.00	1100.00	7.414	596.2	0.7744
600.00	1100.00	6.779	611.1	0.7885
620.00	1100.00	6.318	624.7	0.8012
640.00	1100.00	5.956	637.6	0.8131
660.00	1100.00	5.657	650.1	0.8244
680.00	1100.00	5.403	662.4	0.8352
700.00	1100.00	5.182	674.4	0.8457
720.00	1100.00	4.987	686.3	0.8554
740.00	1100.00	4.813	698.1	0.8652
760.00	1100.00	4.656	709.8	0.8745
780.00	1100.00	4.513	721.5	0.8835
800.00	1100.00	4.382	733.2	0.8923
100.00	1200.00	56.85	112.4	0.1753
200.00	1200.00	56.26	128.4	0.2001
220.00	1200.00	55.62	144.7	0.2214
240.00	1200.00	54.93	161.4	0.2422
260.00	1200.00	54.18	178.5	0.2625
280.00	1200.00	53.37	195.9	0.2824
300.00	1200.00	52.49	213.7	0.3019
320.00	1200.00	51.52	231.6	0.3211
340.00	1200.00	50.48	250.4	0.3393
360.00	1200.00	49.33	269.6	0.3584
380.00	1200.00	48.08	289.2	0.3767

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
2-METHYL PYRIDINE. WATER 35 MOLE PC ORGANIC

E1393 P 13
9/ 1/72

TEMP T DEG F	P PSI	D LB/FT3	H BTU/LB	S BTU/LB-DEG F
400.00	1200.00	46.70	309.4	0.3946
420.00	1200.00	45.18	330.4	0.4121
440.00	1200.00	43.51	352.4	0.4284
460.00	1200.00	41.65	375.6	0.4436
480.00	1200.00	39.58	400.5	0.4576
500.00	1200.00	37.25	428.3	0.4699
520.00	1200.00	34.62	460.9	0.4805
540.00	1200.00	32.30	503.9	0.7214
560.00	1200.00	30.45	552.0	0.7294
580.00	1200.00	28.35	602.4	0.7580
600.00	1200.00	26.11	651.5	0.7771
620.00	1200.00	23.92	706.4	0.7915
640.00	1200.00	21.74	761.0	0.8046
660.00	1200.00	19.46	814.3	0.8166
680.00	1200.00	17.17	867.1	0.8277
700.00	1200.00	14.85	919.6	0.8386
720.00	1200.00	12.51	971.4	0.8491
740.00	1200.00	10.10	1023.9	0.8593
760.00	1200.00	7.71	1075.9	0.8692
780.00	1200.00	5.38	1127.9	0.8784
800.00	1200.00	3.02	1179.7	0.8884
820.00	1500.00	26.85	113.0	0.1774
840.00	1500.00	26.26	129.0	0.1996
860.00	1500.00	25.62	145.3	0.2204
880.00	1500.00	24.93	162.0	0.2415
900.00	1500.00	24.18	179.0	0.2619
920.00	1500.00	23.37	196.3	0.2816
940.00	1500.00	22.49	214.0	0.3011
960.00	1500.00	21.52	232.1	0.3206
980.00	1500.00	20.48	250.6	0.3387
1000.00	1500.00	19.33	269.6	0.3571
1020.00	1500.00	18.08	289.0	0.3751
1040.00	1500.00	16.76	309.1	0.3924
1060.00	1500.00	15.38	329.4	0.4100
1080.00	1500.00	13.91	351.3	0.4254
1100.00	1500.00	12.35	374.1	0.4404
1120.00	1500.00	10.70	398.3	0.4537
1140.00	1500.00	9.05	425.0	0.4661
1160.00	1500.00	7.30	456.2	0.4760
1180.00	1500.00	5.45	495.6	0.4764

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THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 2-METHYLPYRIDINE. WATER 35 MOLE PC ORGANIC

E1793 P 14
 9/ 1/73

TEMP T	D	η	H	S
DEG	PSI	LB/FT ³	BTU/LB	BTU/LB-F
560.00	1500.00	15.96	534.7	0.7691
580.00	1500.00	16.12	543.0	0.7172
600.00	1500.00	16.93	547.8	0.7210
620.00	1500.00	13.34	578.3	0.7504
640.00	1500.00	10.92	603.9	0.7730
660.00	1500.00	9.492	622.4	0.7902
680.00	1500.00	8.881	638.4	0.8047
700.00	1500.00	8.277	653.1	0.8175
720.00	1500.00	7.799	666.9	0.8291
740.00	1500.00	7.404	680.3	0.8404
760.00	1500.00	7.068	693.4	0.8510
780.00	1500.00	6.777	706.2	0.8612
800.00	1500.00	6.520	718.8	0.8710

THERMODYNAMIC PROPERTIES OF SENIOR CANDIDATE FLUIDS
 2-METHYLPYRIDINE, WATER 35 MOLE % ORGANIC

E-393 P 15
 9/ 1/72

THERMODYNAMIC PROPERTIES AT SATURATION

----- BURBLE POINT LIQUID -----				
TEMP	P	ρ	H	S
DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
145.00	5.00	57.78	82.31	0.1405
174.81	10.00	56.94	107.2	0.1767
194.07	14.70	56.38	122.7	0.1940
224.45	25.00	55.46	146.5	0.2289
246.44	50.00	53.91	182.6	0.2723
314.82	100.00	51.78	226.1	0.3109
405.41	300.00	45.30	316.4	0.4051
452.83	500.00	42.34	370.2	0.4451
484.92	700.00	39.03	411.1	0.4676
503.04	900.00	36.23	444.5	0.4770
517.31	1000.00	34.99	459.1	0.4792
525.44	1100.00	33.84	473.0	0.4824
532.94	1200.00	32.72	486.7	0.4751

----- DEW POINT GAS -----				
TEMP	P	ρ	H	S
DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
155.21	5.00	0.3374E-01	482.3	0.8467
189.43	10.00	0.4424E-01	493.9	0.8341
211.23	14.70	0.4180E-01	501.0	0.8279
241.33	25.00	0.1503	511.7	0.8202
246.54	50.00	0.2866	527.5	0.8116
337.81	100.00	0.5503	545.0	0.8057
430.84	300.00	1.619	573.4	0.7979
470.27	500.00	2.848	580.1	0.7824
494.93	700.00	4.402	578.1	0.7601
512.25	900.00	6.814	566.9	0.7513
519.52	1000.00	10.02	546.9	0.7275
526.41	1100.00	11.15	543.9	0.7228
533.21	1200.00	12.30	540.9	0.7183

APPENDIX D

DYNAMIC LOOP TEST PROCEDURE

Before Test

1. Before assembly carefully clean each component and tubing section with acetone and blow dry with compressed nitrogen. The steel heater coil and the aluminum condenser coil are newly fabricated for each test. They should be cleaned with hexane.
2. Assemble loop, observing these precautions:
 - (a) Install new aluminum ferrules in the fittings at each end of the aluminum condensing coil (stainless steel ferrules elsewhere).
 - (b) Install new O-ring seal of specified elastomer in the let-down valve cap and in the sample valve.
 - (c) Renew filter element and PTFE filter seal washer.
3. Check condition and level of Dowtherm A in its boiler. Add or replace as necessary. Level should be no lower than one inch from top.
4. Remove air above Dowtherm A by connecting a vacuum source and evacuating for at least 10 minutes. Leave space evacuated.
5. Evacuate loop by connecting a vacuum pump to valve D (Figure 6, Volume II) with all valves but A open. Test for leaks by watching for pressure rise when the loop is isolated from the pump. Close valve D under high vacuum.
6. Add test fluid to fill glass and bleed into loop by carefully manipulating valve A. Several repetitions are needed, taking care not to let air be drawn in through valve A at any time.
7. Pressurize the fluid in the loop to 20 psig by admitting compressed nitrogen into the top of the part-full fill glass and bleeding sufficient fluid into the loop through valve A. Stopper the fill glass. Close valve C.

Start-up

8. Set the circulating pump for full stroke and turn on.

9. Adjust let-down valve as needed to establish 1000 psig pump discharge pressure.
10. Turn on power to Dowtherm boiler. Set temperature controller.
11. Turn on water to precooler/condenser. Connect 1.5 volt dry cell between aluminum coil and 1 in. x 1 in. magnesium sacrificial anode suspended in water surrounding the coil.
12. Monitor pump suction pressure throughout start-up. As the pressure rises above starting pressure (due to fluid thermal expansion/evaporation), bleed fluid out through valve A into fill glass. Target suction pressure is 20 psig.
13. Adjust pump delivery rate downward only if necessary to achieve final 720°F. heater-out temperature when heat input to boiler is approximately 80% of maximum available.
14. Caution: Valve C should never be opened when the pump suction pressure is higher than 40 psig. Rupture of the vent glass might result. Valve C should never be left open when unattended.
15. Vent whatever gas or vapor appears in the vent glass with valve C open for a minute or two. This should be repeated several times before and after attainment of final temperature equilibrium.
16. Note date and time of initial attainment of 720°F. heater-out temperature. This is taken as test zero time. Upon attainment of satisfactory steady-state operation, close valves B and F to protect the respective pressure gauges from fatigue and overpressure.

Daily Monitoring

17. Note heater-out temperature. Adjust temperature controller set point if necessary to reestablish 720°F. value.
18. Open valve B and check pump discharge pressure. Adjust let-down valve setting if necessary to reestablish 1000 psig.
19. Cautiously open valve F and note pump suction pressure. If above 30 psig, first bleed fluid out through valve A if needed to drop suction pressure to 40 psig, then vent any gas as by step 21. Fluid may then be readmitted through valve A (under compressed nitrogen) if needed to reestablish pump suction pressure.

20. If suction pressure in step 19 was noticeably lower than the reading of a day earlier leakage is a possible reason which should be carefully investigated and corrected. Fluid may then be added to the loop through valve A to restore the suction pressure.
21. Bleed any gas bubbles from the loop by sequential operation of valves C and D. Any gas appearing in the vent glass during the first 4 days of operation may be assumed to be air and discarded. After the first 4 days, all evolved gas is passed through a syringe at ambient conditions and its volume noted.
22. Make entries on run sheet. Collect samples as needed. Leave all valves but E in shut position.

Shutdown

23. Turn off power to Dowtherm A boiler.
24. Turn off pump when heater-out temperature falls below 200°F.
25. When entire system is at or near room temperature, drain the fluid from the loop through valve A after opening valves C and D. Complete drainage requires partial disassembly of the loop and blowing.
26. Measure the pump delivery rate when pumping a higher boiling fluid to 1000 psig at room temperature.
27. Inspect the heater and condenser coils for corrosion and/or deposits.
28. Analyze drained fluid for change from initial condition.

APPENDIX E

ACUTE VAPOR INHALATION REPORT - FINAL CANDIDATE RC-1

Industrial **BIO-TEST** *Laboratories, Inc.*

REPORT TO
MONSANTO COMPANY
ACUTE VAPOR INHALATION TOXICITY STUDY WITH
MFSN 28
IN ALBINO RATS
BTL-72-101
JANUARY 17, 1973
IBT NO. 633-02558

I. Introduction

A sample identified as MFSN 28 was received October 31, 1972, from Monsanto Company for the purpose of conducting an acute vapor inhalation toxicity study using albino rats as experimental animals.

II. Summary

Four groups of ten rats each were used to determine the inhalation median lethal vapor concentration (LC₅₀) of MFSN 28. Each group of animals was exposed to the vapor in a 70-liter inhalation chamber. After exposure, all surviving rats were observed for 14 days.

The acute vapor inhalation median lethal concentration was found to be 115.0 mg/L air (nominal concentration) based on a four-hour period of exposure. Untoward behavioral reactions exhibited by the animals included ataxia, excitation, ptosis, lacrimation, and prostration. Body weight gains of animals surviving the 14-day observation period were normal. Necropsy revealed minimal diffuse red

Industrial **BIO-TEST** *Laboratories, Inc.*

discoloration of the lungs in less than half of the animals tested, however, this is not highly uncommon in rats maintained under laboratory conditions.

Respectfully submitted,

INDUSTRIAL BIO-TEST LABORATORIES, INC.

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III. Procedure

Young adult albino rats (Sprague-Dawley strain*) having an average body weight of 160 grams were employed as test animals. Four groups of ten rats each (five males and five females) were selected after having been under observation for at least five days to insure their general health and suitability for testing. The animals were housed individually in stock cages and permitted a standard laboratory diet** plus water ad libitum, except during inhalation exposure.

Each exposure was designed to run for a four-hour period, during which time observations were made with respect to incidence of mortality and reactions displayed. At the end of the exposure period the rats were returned to their stock cages and observed for the following 14 days.

A body weight was determined for each animal prior to inhalation exposure and for each surviving animal at the end of the 14-day observation period. The data were recorded as an index to body weight effects.

Gross pathologic examinations were scheduled to be conducted upon all animals which might succumb during the test period and upon those sacrificed at the end of the 14-day observation period.

* ARS/Sprague-Dawley, Madison, Wis.

** Purina Rat Chow, Ralston Purina Company, St. Louis, Mo.

Test animals were exposed in a specially constructed Plexiglas inhalation chamber having a capacity of 70 liters. The chamber was designed so that the animals could be introduced to the test atmosphere after 99 percent of the desired vapor concentration was established. Each animal was caged separately during exposure to minimize filtration of inspired air by animal fur.

Vapor was generated by metering, through use of an infusion pump*, the MFSN 28 into a 500 ml flask which was maintained at 120°C. A stream of clean dry air (-40°C dewpoint) was also introduced into this flask and then directed into the exposure chamber at the top center, dispersed by a baffle plate, and exhausted at the bottom. When necessary, additional clean air was added at the top of the chamber to achieve the desired final vapor concentration. The flask and vapor carrying tube were maintained at the desired temperature by a heating jacket and rheostat. Air flow rates through the system were measured with rotameters connected in the air supply lines upstream of vapor contamination. The rotameters were calibrated with a wet-test meter after each exposure was completed. Average nominal vapor concentrations were calculated by dividing the total weight of test material vaporized by the total volume of air used during each inhalation exposure. Temperature and pressure of the test atmosphere were also measured.

*Harvard Syringe Infusion-Withdrawal Pump, Harvard Physiological Apparatus Company, Inc., Dover, Mass.

At the conclusion of the 14-day investigational period, all data were collected and the acute vapor inhalation median lethal concentration (LC_{50}) of the test material was calculated employing the method of Litchfield and Wilcoxon*.

An outline of the test conditions is presented in Table I.

* Litchfield, J. T., Jr. and Wilcoxon, F., "A Simplified Method of Evaluating Dose-Effect Experiments," J. Pharm. & Exp. Ther. 96, 99 (1949).

TABLE I
 TEST MATERIAL: MFSN 28
 Acute Vapor Inhalation Toxicity Study - Albino Rats
 Outline of Test Conditions

Group	Number of Animals Tested	Duration of Exposure (minutes)	Air Delivery Rates (L/min at 29.92 inches Hg and 25°C)			Test Atmosphere Temperature (°C)	Test Atmosphere Pressure (inches Hg)	Average Nominal Vapor Concentration (mg/L air at 29.92 inches Hg and 25°C)	
			Vapor Generator	Additional	Total				
I	10	240	1.3	0	1.3	25	30.18	27.0	
II	10	240	1.6	4.8	6.4	28	29.55	54.9	
III	10	240	1.6	1.5	3.1	29	29.44	90.0	
IV	10	240	1.5	0	1.5	28	29.95	140.2	

IV. Results

A. Mortality

Mortality data and the LC_{50} are presented in Table II.

B. Body Weight Gains

Body weight gains for all surviving animals were within normal limits.

C. Behavioral Reactions

Behavioral reactions exhibited by the animals are listed in Table III.

D. Gross Pathologic Findings

Necropsy revealed minimal diffuse red discoloration of the lungs in less than half the animals tested. This finding is not highly uncommon in rats maintained under laboratory conditions and thus may not be due to inhalation of the test material vapors. There were no gross pathologic alterations in any of the other tissues and organs examined.

TABLE II
TEST MATERIAL: MFSN 28
Acute Vapor Inhalation Toxicity Study - Albino Rats

Mortality Data				
Group	Average Nominal Vapor Concentration (mg/L air)	Number of Animals Tested	Observed Percent Dead	Expected Percent Dead
I	27.0	10	0	0
II	54.9	10	0	0.3
III	90.0	10	0	17.0
IV	140.2	10	100	77.5

Acute Vapor Inhalation LC₅₀ = 115.0 mg/L air (four-hour exposure)
Limits of LC₅₀ at the 95% Level of Confidence = 87.1 - 151.8 mg/L air

TABLE III

TEST MATERIAL: MFSN 28

Acute Vapor Inhalation Toxicity Study - Albino Rats

Reactions

Group	Reactions	Number of Animals Affected	Time of Onset After Start of Exposure	Duration
I	Sneezing	10	10 minutes	4 hours
	Ptosis	10	20 minutes	4 hours
	Hypoactivity	10	30 minutes	4 hours
	Lacrimation	10	40 minutes	5-6 hours
	Prostration	10	2 hours	2 hours
II	Ataxia	10	5 minutes	4 hours
	Excitation	10	10 minutes	5 minutes
	Ptosis	10	15 minutes	4 hours
	Lacrimation	10	15 minutes	5-6 hours
	Prostration	10	15 minutes	4 hours
III	Ataxia	10	5 minutes	4 hours
	Excitation	10	10 minutes	5 minutes
	Ptosis	10	10 minutes	4 hours
	Lacrimation	10	15 minutes	5-6 hours
	Prostration	10	15 minutes	4 hours
IV	Ataxia	10	5 minutes	Until death
	Excitation	10	5-10 minutes	Until death
	Ptosis	10	10 minutes	Until death
	Lacrimation	10	10 minutes	Until death
	Prostration	10	15 minutes	Until death
	Death	10	3-4 hours	

APPENDIX F

ACUTE VAPOR INHALATION REPORT - FINAL CANDIDATE RC-2

Industrial **BIO-TEST** *Laboratories, Inc.*

REPORT TO

MONSANTO COMPANY

ACUTE VAPOR INHALATION TOXICITY STUDY WITH
MFSN 23
IN ALBINO RATS

BTL-72-100

JANUARY 17, 1973

IBT NO. 663-02558

I. Introduction

A sample identified as MFSN 23 was received October 31, 1972, from Monsanto Company for the purpose of conducting an acute vapor inhalation toxicity study using albino rats as experimental animals.

II. Summary

Five groups of ten rats each were used to determine the inhalation median lethal vapor concentration (LC₅₀) of MFSN 23. Each group of animals was exposed to the vapor in a 70-liter inhalation chamber. After exposure, all surviving rats were observed for 14 days.

The acute vapor inhalation median lethal concentration was found to be 14.3 mg/L air (nominal concentration), based on a four-hour period of exposure. Untoward behavioral reactions exhibited by the animals included ptosis, lacrimation, hypoactivity, dyspnea, weakness, ataxia and prostration. Body weight gains of survivors of the 14-day observation period were normal. Necropsy revealed slight diffuse red discoloration

Industrial **BIO-TEST Laboratories, Inc.**

of the lungs in most of the animals which died during the observation period. Approximately half of the animals surviving the 14-day observation period revealed slight diffuse or slight focal red discoloration of the lungs.

Respectfully submitted,

INDUSTRIAL BIO-TEST LABORATORIES, INC.

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III. Procedure

Young adult albino rats (Sprague-Dawley strain*) having an average body weight of 174 grams were employed as test animals. Five groups of ten rats each (five males and five females) were selected after having been under observation for at least five days to insure their general health and suitability for testing. The animals were housed individually in stock cages and permitted a standard laboratory diet** plus water ad libitum, except during inhalation exposure.

Each exposure was designed to run for a four-hour period, during which time observations were made with respect to incidence of mortality and reactions displayed. At the end of the exposure period, the rats were returned to their stock cages and observed for the following 14 days.

A body weight was determined for each animal prior to inhalation exposure and for each surviving animal at the end of the 14-day observation period. The data were recorded as an index to body weight effects.

Gross pathologic examinations were scheduled to be conducted upon all animals which might succumb during the test period and upon those sacrificed at the end of the 14-day observation period.

* ARS/Sprague-Dawley, Madison, Wis.

** Purina Rat Chow, Ralston Purina Company, St. Louis, Mo.

Test animals were exposed in a specially constructed Plexiglas inhalation chamber having a capacity of 70 liters. The chamber was designed so that the animals could be introduced to the test atmosphere after 99 percent of the desired vapor concentration was established. Each animal was caged separately during exposure to minimize filtration of inspired air by animal fur.

Vapor was generated by metering, through use of an infusion pump*, the MFSN 23 into a 500 ml flask which was maintained at 120°C. A stream of clean dry air (-40°C dewpoint) was also introduced into this flask and then directed into the exposure chamber at the top center, dispersed by a baffle plate, and exhausted at the bottom. When necessary, additional clean air was added at the top of the chamber to achieve the desired final vapor concentration. The flask and vapor carrying tube were maintained at the desired temperature by a heating jacket and rheostat. Air flow rates through the system were measured with rotameters connected in the air supply lines upstream of vapor contamination. The rotameters were calibrated with a wet-test meter after each exposure was completed. Average nominal vapor concentrations were calculated by dividing the total weight of test material vaporized by the total volume of air used during each inhalation exposure. Temperature and pressure of the test atmosphere were also measured.

*Harvard Syringe Infusion-Withdrawal Pump, Harvard Physiological Apparatus Company, Inc., Dover, Mass.

Industrial **BIO-TEST** *Laboratories, Inc.*

At the conclusion of the 14-day investigational period, all data were collected and the acute vapor inhalation median lethal concentration (LC_{50}) of the test material was calculated employing the method of Litchfield and Wilcoxon*.

An outline of the test conditions is presented in Table I.

* Litchfield, J. T., Jr. and Wilcoxon, F., "A Simplified Method of Evaluating Dose-Effect Experiments," J. Pharm. & Exp. Ther. 96, 99 (1949).

TABLE I
TEST MATERIAL: MFSN 23
Acute Vapor Inhalation Toxicity Study - Albino Rats

Outline of Test Conditions

Group	Number of Animals Tested	Duration of Exposure (minutes)	Air Delivery Rates (L/min at 29.92 inches Hg and 25°C)			Test Atmosphere Temperature (°C)	Test Atmosphere Pressure (inches Hg)	Average Nominal Vapor Concentration (mg/L air at 29.92 inches Hg and 25°C)	
			Generator	Additional	Total				
I	10	240	1.7	7.5	9.2	30	29.55	8.6	
II	10	240	5.0	9.1	14.1	29	29.93	10.5	
III	10	240	1.8	3.0	4.8	30	29.45	16.2	
IV	10	240	1.7	4.1	5.8	30	29.62	19.4	
V	10	240	2.0	2.9	4.9	26	30.10	25.3	

IV. Results

A. Mortality

Mortality data and the LC_{50} are presented in Table II.

B. Body Weight Effects

The average two-week body weight gain for all surviving animals in each group was within normal limits.

C. Behavioral Reactions

Behavioral reactions exhibited by the animals are listed in Table III.

D. Gross Pathologic Findings

Necropsy of rats which died during the exposure or the 14-day observation period revealed slight diffuse red discoloration of the lungs. Slight diffuse or focal red discoloration of the lungs was found in about half of the animals which survived the observation period. All other animals showed no gross pathologic alterations in any of the tissues and organs examined.

TABLE II
TEST MATERIAL: MFSN 23
Acute Vapor Inhalation Toxicity Study - Albino Rats

Mortality Data				
Group	Average Nominal Vapor Concentration (mg/L air)	Number of Animals Tested	Observed Percent Dead	Expected Percent Dead
I	8.6	10	0	0.42
II	10.5	10	20	6.00
III	16.2	10	60	74.00
IV	19.4	10	100	95.00
V	25.3	10	100	99.88

Acute Vapor Inhalation LC₅₀ = 14.3 mg/L air (four-hour exposure)
Limits of LC₅₀ at the 95% Level of Confidence = 12.0 - 17.0 mg/L air

TABLE III

TEST MATERIAL: MFSN 23

Acute Vapor Inhalation Toxicity Study - Albino Rats

Reactions

Group	Reactions	Number of Animals Affected	Time of Onset After Start of Exposure	Duration
I	Ptosis	10	50 minutes	5-8 hours
	Lacrimation	10	50 minutes	5-8 hours
	Hypoactivity	10	50 minutes	12-18 hours
	Ataxia	10	2 hours	4-5 hours
	Prostration	10	3 hours	4-5 hours
II	Ptosis	10	30 minutes	5-8 hours
	Lacrimation	10	30 minutes	5-8 hours
	Hypoactivity	10	30 minutes	12-18 hours
	Prostration	10	150 minutes	4-5 hours
	Death	2	4-8 hours	
III	Ptosis	10	30 minutes	5-8 hours
	Lacrimation	10	30 minutes	5-8 hours
	Hypoactivity	10	30 minutes	12-18 hours
	Prostration	10	90 minutes	5-6 hours
	Death	6	3-8 hours	
IV	Ptosis	10	15 minutes	Until death
	Lacrimation	10	15 minutes	Until death
	Hypoactivity	10	20 minutes	Until death
	Dyspnea	10	20 minutes	Until death
	Prostration	10	30 minutes	Until death
	Death	10	3 hours	
V	Ptosis	10	10 minutes	Until death
	Lacrimation	10	15 minutes	Until death
	Hypoactivity	10	20 minutes	Until death
	Dyspnea	10	20 minutes	Until death
	Prostration	10	45 minutes	Until death
	Death	10	3 hours	

APPENDIX G

ACUTE VAPOR INHALATION REPORT - HEXAFLUOROBENZENE/PENTAFLUOROBENZENE

ACUTE INHALATION TOXICITY OF
HEXAFLUOROBENZENE, PENTAFLUOROBENZENE
AND A 50:50 MIXTURE

by
R A Riley
January, 1973

(For the Imperial Smelting Corporation Limited)

SUMMARY

The acute (30 minute) LC50 in the mouse of hexafluorobenzene is 6-7%, pentafluorobenzene is 2-3%, and a 50:50 mixture of the two is 4-6%. Synergism does not occur in the mixture.

The samples of hexafluorobenzene and pentafluorobenzene were supplied by Imperial Smelting Corporation.

METHODS

Groups of 10 female mice of the Alderley Park specific pathogen free, albino strain (body weights 25-30 g) were used. They were exposed to dynamic atmospheres of the chemicals, for a period of 30 minutes, in a small exposure chamber of 40 litres capacity, and observed for a further seven days.

The atmospheres were generated by a syringe and atomiser technique, and the atmospheric concentrations checked by gas chromatography.

RESULTS

The mortality data are tabulated below:

	Dose (volume %) and mortality						
	2	3	4	5	6	7	8
Hexafluorobenzene	-	-	-	-	3/10	6/10	10/10
Pentafluorobenzene	2/10	8/10	7/10	9/10	-	-	-
50:50 mixture	-	-	4/10	-	6/10	-	9/10

From the above figures the acute (30 minute) LC50 of hexafluorobenzene is estimated to be 6-7%, pentafluorobenzene 2-3% and the 50:50 mixture 4-6%.

The animals in each experiment showed similar toxic signs in that they became comatose within a few minutes and died following a period of profound respiratory depression. The survivors from the higher doses took up to two days to recover fully from the effects of exposure.

Using the mean harmonic formula it can be calculated that a 50:50 mixture of the two chemicals should have an acute LC50 of approximately 3.5% provided

that their toxic effects are additive. The observed value of 4-6% therefore shows that synergism has not occurred.

DGC/AMR
4 Jan 72

APPENDIX H

TOXICITY AND BIODEGRADABILITY OF PYRIDINES - LITERATURE ABSTRACTS

The following references relating to toxicity and/or biodegradability of various pyridine fluids appeared to be pertinent to present considerations regarding acceptability of methylpyridine-water working fluids. The published data, which are somewhat fragmentary, cover 2-methyl pyridine more completely than the others. Extracts and sources follow.

1. 2-Methylpyridine (alpha picoline)

(a) Acute Oral Toxicity:

LD₅₀ = 674 mg/kg in mice
790 mg/kg in rats
900 mg/kg in guinea pigs

Ref: V.G. Veselov, *Mater. Nauch.-Proct. Konf. Molodykh Gig. Sanit. Urachei*, 11th 1967, 121, *Chem. Abstr.* 72, 41134 (1970).

(b) Chickens given 20 g 2-methylpyridine subcutaneously converted the material to α -pyridineornithuric acid which is eliminated in the urine.

Ref. S. Tsunoo, et al., *Japan J. Pharmacol.*, 15, 149 (1965).
Chem. Abstr. 63, 12150 (1965).

(c) The single dose oral LD₅₀ in rats for 2-methylpyridine is 1.41 g/kg body weight.

Ref. H. F. Smyth, Jr., et al., *Arch. Ind. Hyg. Occupational Med.* 4, 119 (1951). *Chem. Abstr.* 45, 9710 (1951).

(d) Toxicity parameters for rats have been given as:

LD₀ = 550; LD₅₀ = 790 and, LD₁₀₀ = 950 mg/kg.

Ref. S.A. Polilei, et al., *Nauch. Tr., Omsk. Med. Inst.* 1969, No. 88, 319. *Chem. Abstr.* 75, 107,789 (1971).

(e) α -Picoline and 2,5-lutidine were highly stable in aqueous solutions and aggravated organoleptic properties of H₂O, with threshold concentrations, equal to 1.32 and 0.47 mg/l, respectively. At concentrations >1 mg/l, both inhibited self-purification of the H₂O. Acute experiments on mice, rats, and guinea pigs showed that α -picoline was the more toxic (av. LD = 790 mg/kg in rats, compared

to 800 mg/kg for 2,5-lutidine). Chronic sanitary-toxicological experiments (180 days administration) showed that doses corresponding to the average tolerable concentration of pyridine in reservoirs (0.2 mg/l) caused α -picoline and 2,5-lutidine toxicity (decreased cholinesterase and increased prothrombin activity, reduced the concentrating ability of the kidney, and weakened central nervous system excitation). The maximum nonactive dose of the two compounds was 2.5×10^{-3} mg/kg which corresponds to 0.05 mg/l, suggesting that this is the maximum permissible concentration for both α -picoline and 2,5-lutidine in bodies of water.

Ref. V. G. Veselov, (Omsk, Med. Inst. im. Kalinina, Omsk USSR). *Gig. Sanit.* 1968, 33(12), 18-22 (Russ.), Biological Action and the Hygienic Significance of α -Picoline and 2,5-Lutidine in Water Reservoir Contamination. *Chem. Abstr.* 70, 45795z (1969).

2. 4-Methylpyridine (gamma picoline)

The single dose oral LD₅₀ in rats was given as 1.29 g/kg (same reference as under 1c above).

3. Methylpyridines (picolines)

Microorganisms belonging to various taxonomic groups and utilizing 2-, 3-, and 4-methylpyridine and 5-ethylpyridine as the sole source of C were studied. Over 100 cultures of *Mycobacterium*, *Nocardia*, and others caused the opening of the pyridine ring and oxidation of alkyl substitutes, followed by pyridine ring metabolism. Oxidation of the Me group of 3-methylpyridine to a carboxyl group was established. A method of microbiological production of nicotinic acid in 80% yield using 3-methylpyridine was elaborated.

Ref. G. K. Skryabin, L. A. Golovleva, B. I. Krupyanko, (Inst. Biokhim, Fiziol. Mikroorganizmov, Moscow, USSR), Microbiological Transformation of Pyridine Compounds, *Izv. Akad. Nauk SSSR, Ser. Biol.* 1969 (5), 660-9 (Russ). *Chem. Abstr.* 72, 10084f (1970).

4. Pyridine

(a) Subcutaneous injection in rats gave the following LD₅₀ = 1.0 g/kg.

Ref. F. G. Brazda and R. A. Coulson, *Proc. Soc. Exptl. Biol. Med.* 62, 19 (1946). *Chem. Abstr.* 40 4799 (1946).

(b) Pyridine administered to dogs and rabbits is rapidly eliminated mostly through the skin, lungs, and feces and a small amount in the urine as free pyridine.

Ref. N. J. Novello, *J. Biol. Chem.* 74 33 (1927). *Chem. Abstr.* 27, 2746 (1933).

(c) Pyridine has a "feeble" effect on fish at a concentration of 1 part in 1000.

Ref. V. Demyanenko, *Ilig. i. Epidem. (USSR)* 10, No. 6/7, 13 (1931); Dept. Sci. Ind Res (Brit.), Water Pollution Research, Summary of Current Lit. 6, 35. *Chem. Abstr.* 27, 2746 (1933).

(d) Rats given diets containing 0.6% of pyridine or 1% of quinoline (as acetates) for 28 days showed enlarged livers with abnormally high water content. Cystine or methionine added to the ration exerted an important protective action but choline gave very little protection. Isoquinoline also produced liver damage.

Ref. Roland A. Coulson and Fred G. Brazda, Influence of Choline, Cystine, and Methionine on Toxic Effects of Pyridine on Certain Related Compounds, *Proc. Soc. Exptl. Biol. Med.* 69, 480-7 (1948); (*cf* C.A. 42, 3861f.) *Chem. Abstr.* 43, 2321h (1949).

(e) No toxic symptoms were noted after administration of 0.31-1.54 cc of pyridine per day to men. In larger doses, 1.85-2.46 cc, the pyridine was toxic, causing one death. Symptoms of hepatorenal disease were noted.

Ref. Lewis J. Pollock, Isidore Finkelman and Alex J. Arieff, Toxicity of Pyridine in Man, *Arch. Internal Med.* 71, 95-106 (1943). *Chem. Abstr.* 37, 4468³ (1943).

The following two references establish the biodegradability of pyridine.

(f) Species of *Proactinomyces* are obtained in soil enriched with 0.1% pyridine (I). Pure cultures of the organisms utilize I as the sole source of C and N. HN_3 and oxalic acid were found as products of the breakdown.

Ref. F. W. Moore, Utilization of Pyridine by Microorganisms, *J. Gen. Microbiol.* 3, 143-9 (1949). *Chem. Abstr.* 43, 4329H (1949).

(g) Batch experiments with activated sludge in which sewage and solutions with 50-6000 mg $\text{C}_5\text{H}_5\text{N}$ (I)/l were added, have achieved complete removal of I in concentrations up to 3000 mg/l after 16 hr of detention time and with a load up to 3000 mg I/l of aeration tank/day. Shock increase of load causes deterioration of the

effluent which improves for concentrations below 3000 mg/l within 10 days, but is impaired above 3000 mg/l. Activated sludge, fed with 2360 and 4760 mg I/l of tank/day, having 1 mg PO₄-P/100 mg of 5-day B.O.D. added, removes all the I and 3 hr of detention. The mean value of 5-day B.O.D. from 54 analyses is 1.2 g O/g of I.

Ref. Alexander Grunwald (VSCHT, Prague, Czech.), Effect of Pyridine on the Activated Sludge Process, *Sb. Vys. Sk. Chem.-Technol. Praze, Technol. Vody*. 1968, 13, 15-26 (Czech). *Chem. Abstr.* 70, 70914v (1969).

APPENDIX I

ACUTE TOXICOLOGICAL INVESTIGATION OF ADVANCED CANDIDATE WORKING FLUIDS

Results of acute toxicity tests performed by Younger Laboratories, St. Louis, are given in a series of tables following. Tests were made using a group of advanced working fluid candidates as defined in Table I-1.

Table I-1. GUIDE TO TEST RESULTS

Fluid Composition				Table Number of Test Report			
				Rat	Rabbit		
Fluid	Mol %A	Component A	Component B	Oral LD ₅₀	Skin MLD	Skin Irr.	Eye Irr.
RC-1	60	Pentafluoro- benzene	Hexafluoro- benzene	I-2	I-3	I-4	I-5
RC-2	60	Water	2-Methylpyri- dine	I-6	I-7	I-8	I-9, 10
MFSN-21	60	Water	3-Methylpyri- dine	I-11	I-12	I-13	I-14, 15
MFSN-24	60	Water	4-Methylpyri- dine	I-16	I-17	I-18	I-19, 20
FSN-106	100	4-Methylpyri- dine	--	I-21	I-22	I-23	I-24, 25
MFSN-27	60	Pentafluoro- pyridine	Hexafluoro- benzene	I-26	I-27	I-28	I-29, 30

Test experimental procedures are summarized as follows:

(A) Oral LD₅₀ (Rats, Mixed Sex)

The undiluted compound was fed by stomach tube to Sprague-Dawley strain albino male and female rats.

After the approximate minimal Lethal Dose was determined, groups of male and female rats were fed in increasing doses at increments of 0.1 fractional log intervals at four levels designed to

blanket the toxicity range thereby supplying data for calculation of the LD₅₀ which was done according to the method of E. J. de Beer.

Observations were made for toxic signs and the viscera of the test animals were examined macroscopically.

(B) Acute Skin Absorption Minimal Lethal Dose
(Rabbits, Mixed Sex)

The undiluted compound was applied in increasing doses at increments of various fractional log intervals to the closely clipped, intact skin of New Zealand white male and female rabbits.

The treatment areas were covered with plastic strips and the animals held in wooden stocks for periods up to 24 hours, after which time they were assigned to individual cages.

Observations were made for toxic signs and the viscera of the test animals were examined macroscopically.

(C) Skin Irritation (Rabbits, Mixed Sex)

0.2 Milliliter of undiluted sample was applied to the clipped, intact skin of New Zealand white male and female rabbits under a one inch by one inch square patch, two single layers thick. The patches were held in place with adhesive tape. The trunk of each animal was wrapped with plastic strips, to retard evaporation and avoid contamination, for the 24 hour exposure period.

Observations were made over a period of seven days for irritation.

The data were scored according to the method of Draize, Woodard and Calvery (Journal of Pharm. and Exp. Therapeutics, Volume 82, December, 1944).

(D) Eye Irritation (Rabbits, Mixed Sex)

0.1 Milliliter of undiluted sample was placed in the conjunctival sac of the right eye of each of two groups of three albino male and female rabbits and observations made over a period of seven days for inflammation.

The eyes were rinsed with warm isotonic saline solution after:
(a) 24 hours exposure, and (b) 15 minutes exposure.

The left eye served as a control.

The data were scored according to the method of Draize, et al.

Table I-2. THE ACUTE ORAL MINIMAL LETHAL DOSE OF RC-1 FOR RATS
Sample Fed Undiluted

<u>Animal No. & Sex</u>	<u>Weight grams</u>	<u>Dose Mg./Kg.</u>	<u>Fate</u>
1-female	215	10,000	survived
2-male	210	10,000	survived
3-female	235	10,000	survived
4-male	215	10,000	survived
5-female	215	10,000	survived
6-male	200	12,600	survived
7-female	225	12,600	survived
8-male	205	12,600	survived
9-female	215	12,600	survived
10-male	240	12,600	died
11-female	220	15,800	died
12-male	200	15,800	died
13-female	225	15,800	died
14-male	210	15,800	died
15-female	210	15,800	survived

DISCUSSION

The Acute Oral Minimal Lethal Dose for male and female rats was found to be greater than 10,000 milligrams per kilogram and less than 12,600 milligrams per kilogram.

The compound was classed as practically non-toxic by oral ingestion in male and female rats.

Survival time was 1 - 5 days with most deaths occurring within two days.

Toxic signs included reduced appetite and activity and lethargy (one to four days in survivors), increasing weakness, slight tremors, ocular discharge, collapse, and death.

At autopsy there was hemorrhagic areas of the lungs, slight liver discoloration, and acute gastrointestinal inflammation.

Surviving animals were sacrificed seven days after dosing. The viscera appeared normal by macroscopic examination.

Table I-3. THE ACUTE SKIN ABSORPTION MINIMAL
LETHAL DOSE OF RC-1 FOR RABBITS

Sample Applied Undiluted

<u>Animal No.-Sex</u>	<u>Weight Kg.</u>	<u>Dose Mg.-Kg.</u>	<u>Animal Weight 5 Days Later Kg.</u>	<u>Fate</u>
1-male	2.5	2000	+0.1	survived
2-female	2.2	3160	+0.1	survived
3-male	2.4	5010	0.0	survived
4-female	2.3	7940	+0.1	survived
5-male	2.5	7940	+0.2	survived

DISCUSSION

The Acute Skin Absorption Minimal Lethal Dose for male and female rabbits was found to be greater than 7940 milligrams per kilogram.

The compound was classed as practically non-toxic by skin absorption in male and female rabbits.

There was no weakness or other outward signs of systemic toxicity.

Surviving animals were sacrificed 14 days after dosing. The viscera appeared normal by macroscopic examination.

Table I-4. SKIN IRRITATION IN RABBITS AFTER APPLICATION OF RC-1

Sample (0.5 milliliter) Applied Undiluted

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	0	2	2	0	0	0
2-female	0	4	2	0	0	0
3-male	0	3	1	0	0	0
Average	0.0	3.0	1.6	0.0	0.0	0.0

DISCUSSION

The compound was classed as a moderate irritant when applied undiluted to intact skin of male and female rabbits.

The average maximum score was 3.0 out of a possible 8 in 24 hours.

Observations following application --

1-hour	No skin changes; zero readings
24-hours	Very slight to slight erythema and edema
48-hours	Very slight erythema, very slight edema in two instances
72-hours	No erythema or edema; zero readings
120-168 hours	No erythema or edema; zero readings

Table I-5. EYE IRRITATION IN RABBITS AFTER APPLICATION OF RC-1

Sample (0.1 milliliter) Applied Undiluted

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	12	2	0	0	0	0
2-female	8	2	0	0	0	0
3-male	10	2	0	0	0	0
Average	10.0	2.0	0.0	0.0	0.0	0.0

DISCUSSION

The compound was classed as a slight eye irritant in male and female rabbits. The average maximum score was 10.0 out of a possible 110 in one hour.

Observations following application --

Immediate	Discomfort was moderate to severe with blinking, pawing, and the eyes tightly closed
10-minutes	Slight to moderate erythema, slight edema, copious discharge
1-hour	Slight to moderate erythema, very slight edema, moderate to copious discharge
24-hour	Slight erythema; no edema or discharge
48-hour	Eyes normal; zero readings
72-168-Hour	Eyes normal; zero readings

Table I-6. THE ORAL LD₅₀ OF RC-2 FOR RATS

Sample Fed Undiluted

<u>Animal No. & Sex</u>	<u>Weight grams</u>	<u>Dose Mg./Kg.</u>	<u>Fate</u>
1-female	230	631	survived
2-male	210	631	survived
3-female	215	631	survived
4-male	220	631	survived
5-female	205	631	survived
6-male	255	794	survived
7-female	230	794	survived
8-male	260	794	died
9-female	240	794	survived
10-male	230	794	survived
11-female	245	1000	survived
12-male	240	1000	died
13-female	215	1000	died
14-male	215	1000	survived
15-female	220	1000	survived
16-male	220	1260	died
17-female	200	1260	died
18-male	250	1260	died
19-female	220	1260	died
20-male	270	1260	died

DISCUSSION

The Oral LD₅₀ for male and female rats was placed at 810 milligrams per kilogram with lower and upper limits of 730 to 910 milligrams per kilogram.

The compound was classed as mildly toxic by oral ingestion in male and female rats.

Survival time was one to three days.

Toxic signs included reduced appetite and activity (one to three days in survivors), increasing weakness, ocular discharge containing blood, collapse, and death.

At autopsy there was hemorrhagic lungs, liver discoloration, and acute gastrointestinal inflammation.

Surviving animals were sacrificed seven days after dosing. The viscera appeared normal by macroscopic examination.

Table I-7. THE ACUTE SKIN ABSORPTION MINIMAL
LETHAL DOSE OF RC-2 FOR RABBITS

Sample Applied Undiluted

Animal No. & Sex	Weight Kg.	Dose Mg./Kg.	Weight Change 5 Days Later Kg.	Fate
1-female	2.8	79.4	0.0	survived
2-male	2.6	200.0	+0.1	survived
3-female	2.5	316.0	--	died - 1 da
4-male	2.7	501.0	--	died - 1 da
5-female	2.6	1000.0	--	died - 16 hr
6-male	2.6	2000.0	--	died - 16 hr

DISCUSSION

The Acute Skin Absorption Minimal Lethal Dose for male and female rabbits was found to be greater than 200 milligrams per kilogram and less than 316 milligrams per kilogram.

The compound was classed as moderately toxic by skin absorption in male and female rabbits.

Survival time was 16 hours to one day.

Toxic signs included reduced appetite and activity (1-3 days in survivors), rapidly increasing weakness, collapse, and death.

At autopsy there was hemorrhagic lungs, slight liver discoloration, and gastrointestinal inflammation.

Surviving animals were sacrificed 14 days after dosing. The viscera appeared normal by macroscopic examination.

Table I-8. SKIN IRRITATION IN RABBITS AFTER APPLICATION OF RC-2

Sample (0.2 milliliter) Applied Undiluted

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-female	0	5	4	3	1	0
2-male	0	6	5	3	1	0
3-female	0	6	4	3	0	0
Average	0.0	5.6	4.3	3.0	0.6	0.0

DISCUSSION

The compound was classed as a severe irritant when applied undiluted to intact skin of male and female rabbits.

The average maximum score was 5.6 out of a possible 8 in 24 hrs.

Observations following application --

1-hour	No skin changes; zero readings
24-hours	Moderate erythema, slight to moderate edema
48-hours	Slight to moderate erythema, slight edema
72-hours	Slight erythema, very slight edema
120-hours	Very slight erythema in two instances; no edema
168-hours	No erythema or edema; zero readings

Note: Sample had a defatting effect on the skin causing the skin to flake off in 10-14 days. There was no injury in depth.

Table I-9. EYE IRRITATION IN RABBITS AFTER APPLICATION OF RC-2

Sample (0.1 milliliter) Applied Undiluted - 24 hours exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-female	58	66	64	50	44	40
2-male	64	71	67	50	40	27
3-female	56	76	70	48	38	30
Average	59.3	71.0	67.0	49.3	40.6	32.3

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 71.0 out of a possible 110 in 24 hours.

Observations following application --

Immediate	Discomfort was moderate with pawing and the eyes tightly closed
10-minutes	Slight corneal dullness, moderate to severe erythema, slight edema, copious discharge
1-hour	Translucent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, slight to moderate edema, copious discharge
24-hours	Translucent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, slight to moderate edema, copious discharge containing whitish exudate
48-120-hours	Gradual improvement
168-hours	Diffuse to translucent areas of corneal cloudiness, slight erythema in one instance; no edema or discharge
10-days	Barely perceptible areas of corneal cloudiness in two instances
14-days	Eyes normal; zero readings

Table I-10. EYE IRRITATION IN RABBITS AFTER APPLICATION OF RC-2

Sample (0.1 milliliter) Applied Undiluted - 15 minutes exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	68	69	30	24	7	0
2-female	66	49	24	22	10	0
3-male	60	54	35	20	5	0
Average	64.6	57.3	29.6	22.0	7.3	0.0

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 64.6 out of a possible 110 in one hour.

Observations following application --

Immediate	Discomfort was moderate with pawing and the eyes tightly closed
10-minutes	Slight corneal dullness, moderate to severe erythema, slight edema, copious discharge
1-hour	Opalescent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, moderate edema, copious discharge
24-hours	Opalescent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, moderate edema, copious discharge containing whitish exudate
48-120-hours	Gradual improvement
168-hours	Eyes normal; zero readings

Table I-11. THE ORAL LD₅₀ OF MFSN-21 FOR RATS

Sample Applied Undiluted

<u>Animal No. & Sex</u>	<u>Weight gram</u>	<u>Dose Mg./Kg.</u>	<u>Fate</u>
1-female	210	501	survived
2-male	205	501	died
3-female	260	501	survived
4-male	260	501	survived
5-female	210	501	survived
6-male	260	631	survived
7-female	215	631	survived
8-male	210	631	died
9-female	230	631	survived
10-male	220	631	died
11-female	200	794	died
12-male	235	794	died
13-female	225	794	survived
14-male	250	794	died
15-female	205	794	survived
16-male	200	1000	died
17-female	210	1000	survived
18-male	240	1000	died
19-female	210	1000	died
20-male	240	1000	died

DISCUSSION

The Oral LD₅₀ for male and female rats was placed at 710 milligrams per kilogram with lower and upper limits of 620 to 820 milligrams per kilogram.

The compound was classed as mildly toxic by oral ingestion in male and female rats.

Survival time was one to four days with most deaths occurring within three days.

Toxic signs included reduced appetite and activity (for one to four days in survivors), ocular discharge containing blood, increasing weakness, collapse, and death.

At autopsy there was hemorrhagic lungs, liver discoloration, and acute gastrointestinal inflammation.

Surviving animals were sacrificed seven days after dosing. The viscera appeared normal by macroscopic examination.

Table I-12. THE ACUTE SKIN ABSORPTION MINIMAL
LETHAL DOSE OF MFSN-21 FOR RABBITS

Sample Applied Undiluted

Animal No. & Sex	Weight Kg.	Dose Mg./Kg.	Weight Change 5 Days Later Kg.	Fate
1-male	2.8	79.4	+0.1	survived
2-female	2.5	126.0	+0.1	survived
3-male	2.8	200.0	-0.1	died - 6 da
4-female	2.7	316.0	0.0	survived
5-male	2.5	501.0	--	died - 3 da
6-female	2.4	1000.0	--	died - 4 da
7-male	2.2	2000.0	--	died - 1 da

DISCUSSION

The Acute Skin Absorption Minimal Lethal Dose for male and female rabbits was found to be greater than 126 milligrams per kilogram and less than 200 milligrams per kilogram.

The compound was classed as highly toxic by skin absorption in male and female rabbits.

Survival time was one to six days.

Toxic signs included reduced appetite and activity (1-3 days in survivors), increasing weakness, collapse, and death.

At autopsy there was hemorrhagic lungs, slight liver discoloration, and gastrointestinal inflammation.

Surviving animals were sacrificed 14 days after dosing. The viscera appeared normal by macroscopic examination.

Table I-13. SKIN IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-21

Sample (0.2 milliliter) Applied Undiluted

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	0	5	4	1	0	0
2-female	0	5	3	1	0	0
3-male	0	5	4	2	0	0
Average	0.0	5.0	3.6	1.3	0.0	0.0

DISCUSSION

The compound was classed as a severe irritant when applied undiluted to intact skin of male and female rabbits.

The average maximum score was 5.0 out of a possible 8 in 24 hrs.

Observations following application --

1-hour	No skin changes; zero readings
24-hours	Slight erythema, moderate edema
48-hours	Slight erythema, slight to moderate edema
72-hours	Very slight erythema, very slight edema in one instance
120-hours	No erythema or edema; zero readings
168-hours	No erythema or edema; zero readings

Note: Sample had a defatting effect on the skin causing the skin to flake off in 10-14 days. There was no injury in depth.

Table I-14. EYE IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-21

Sample (0.1 milliliter) Applied Undiluted -- 24 hr exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-female	56	71	67	48	42	25
2-male	71	73	65	63	27	15
3-female	58	58	56	52	31	27
Average	61.6	67.3	62.6	54.3	33.3	22.3

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 67.3 out of a possible 110 in 24 hours.

Observations following application --

Immediate	Discomfort was moderate with pawing and the eyes closed
10-minutes	Slight corneal dullness, moderate erythema, very slight to slight edema, copious discharge
1-hour	Easily discernable to translucent film over cornea, iris showed little or no reaction to light, moderate to severe erythema, slight to moderate edema, copious discharge
24-hours	Translucent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, moderate edema, copious discharge containing whitish exudate
48-120-hours	Gradual improvement
168-hours	Diffuse to easily discernable areas of Corneal cloudiness, iris reaction to light was sluggish, slight erythema in one instance; no edema or discharge
10-days	Eyes normal; zero readings

Table I-15. EYE IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-21

Sample (0.1 milliliter) Applied Undiluted -- 15-min exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-female	59	59	24	24	12	5
2-male	71	73	41	31	10	0
3-female	59	53	34	22	10	0
Average	63.0	65.0	33.0	25.6	10.6	1.6

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 65.0 out of a possible 110 in 24 hours.

Observations following application --

Immediate	Discomfort was moderate with pawing and the eyes closed
10-minutes	Slight corneal dullness, moderate erythema, slight edema, copious discharge
1-hour	Opalescent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, moderate edema, copious discharge
24-hours	Opalescent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, moderate edema, copious discharge containing whitish exudate
48-hours	Gradual improvement
72-120-hours	Gradual improvement
168-hours	Very slight diffuse areas of corneal cloudiness in one instance
10-days	Eyes normal; zero readings

Table I-16. THE ORAL LD₅₀ OF MFSN-24 FOR RATS

Sample Fed Undiluted

<u>Animal No. & Sex</u>	<u>Weight gram</u>	<u>Dose Mg./Kg.</u>	<u>Fate</u>
1-female	235	631	died
2-male	225	631	survived
3-female	260	631	survived
4-male	210	631	survived
5-female	205	631	survived
6-male	235	794	died
7-female	205	794	survived
8-male	250	794	died
9-female	235	794	survived
10-male	210	794	survived
11-female	225	1000	died
12-male	210	1000	survived
13-female	215	1000	died
14-male	265	1000	died
15-female	200	1000	survived
16-male	210	1260	died
17-female	200	1260	died
18-male	215	1260	died
19-female	220	1260	died
20-male	200	1260	died

DISCUSSION

The Oral LD₅₀ for male and female rats was placed at 700 milligrams per kilogram with lower and upper limits of 620 to 800 milligrams per kilogram.

The compound was classed as mildly toxic by oral ingestion in male and female rats.

Survival time was one to three days with most deaths occurring within two days.

Toxic signs included reduced appetite and activity (for one to three days in survivors), ocular discharge containing blood, increasing weakness, collapse, and death.

At autopsy there was hemorrhagic lungs, liver discoloration, and acute gastrointestinal inflammation.

Surviving animals were sacrificed seven days after dosing. The viscera appeared normal by macroscopic examination.

Table I-17. THE ACUTE SKIN ABSORPTION MINIMAL
LETHAL DOSE OF MFSN-24 FOR RABBITS

Sample Applied Undiluted

<u>Animal No. & Sex</u>	<u>Weight Kg.</u>	<u>Dose Mg./Kg.</u>	<u>Weight Change 5 Days Later Kg.</u>	<u>Fate</u>
1-male	2.7	79.4	0.0	survived
2-female	2.1	126.0	+0.1	survived
3-male	2.5	200.0	-0.1	survived
4-female	2.6	316.0	--	died - 1 da
5-male	2.7	501.0	--	died - 16 hr
6-female	2.6	1000.0	--	died - 16 hr
7-male	2.0	2000.0	--	died - 12 hr

DISCUSSION

The Acute Skin Absorption Minimal Lethal Dose male and female rabbits was found to be greater than 200 milligrams per kilogram and less than 316 milligrams per kilogram.

The compound was classed as moderately toxic by skin absorption in male and female rabbits.

Survival time was 12 hours to one day.

Toxic signs included reduced appetite and activity and slight lethargy (1-2 days in survivors), rapidly increasing weakness, collapse, and death.

At autopsy there was hemorrhagic lungs and slight liver discoloration.

Surviving animals were sacrificed 14 days after dosing. The viscera appeared normal by macroscopic examination.

Table I-18. SKIN IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-24

Sample (0.2 milliliter) Applied Undiluted

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-female	0	5	4	3	1	0
2-male	0	4	4	1	1	0
3-female	0	5	4	2	1	0
Average	0.0	4.6	4.0	2.0	1.0	0.0

DISCUSSION

The compound was classed as a severe irritant when applied undiluted to intact skin of male and female rabbits.

The average maximum score was 4.6 out of a possible 8 in 24 hrs.

Observations following application --

1-hour	No skin changes; zero readings
24-hours	Slight erythema, slight to moderate edema
48-hours	Slight erythema and edema
72-hours	Very slight to slight erythema, very slight edema in one instance
120-hours	Very slight erythema; no edema
168-hours	No erythema or edema; zero readings

Note: Sample had a defatting effect on the skin causing the skin to flake off in 10-14 days. There was no injury in depth.

Table I-19. EYE IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-24

Sample (0.1 milliliter) Applied Undiluted -- 24 hrs exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	61	88	82	63	59	42
2-female	71	71	65	59	57	40
3-Male	54	71	67	61	42	25
Average	62.0	76.6	71.3	61.0	52.6	35.6

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 76.6 out of a possible 110 in 24 hours.

Observations following application --

Immediate	Discomfort was moderate with pawing and the eyes closed tightly
10-minutes	Slight corneal dullness, moderate erythema, slight edema, copious discharge
1-hour	Easily discernable translucent film over cornea, iris reaction to light was sluggish, moderate erythema, slight to moderate edema, copious discharge
24-hours	Opalescent to opaque areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, slight to moderate edema, copious discharge containing whitish exudate
48-120-hours	Gradual improvement
168-hours	Translucent to opalescent areas of corneal cloudiness, iris reaction to light was sluggish, slight erythema in one instance; no edema or discharge
10-days	Barely perceptible areas of corneal cloudiness in one instance
14-days	Eyes normal; zero readings

Table I-20. EYE IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-24

Sample (0.1 milliliter) Applied Undiluted -- 15 min exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	41	71	33	33	17	0
2-female	66	71	65	50	27	10
3-male	55	61	48	31	17	0
Average	54.0	67.6	48.6	38.0	20.3	3.3

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 67.6 out of a possible 110 in 24 hours.

Observations following application --

Immediate	Discomfort was moderate with pawing and the eyes tightly closed
10-minutes	Slight corneal dullness, moderate erythema, slight edema, copious discharge
1-hour	Barely perceptible to slight film over cornea, iris reaction to light was sluggish, moderate erythema and edema, copious discharge
24-hours	Opalescent areas of corneal cloudiness, iris showed no reaction to light, moderate, erythema and edema, copious discharge containing slight whitish exudate
48-120-hours	Gradual improvement
168-hours	Barely perceptible areas of corneal cloudiness in one instance
10-days	Eyes normal; zero reading

Table I-21. THE ORAL LD₅₀ OF FSN-106 FOR RATS

Sample Fed Undiluted

<u>Animal No. & Sex</u>	<u>Weight Gram</u>	<u>Dose Mg./Kg.</u>	<u>Fate</u>
1-female	215	501	survived
2-male	230	501	survived
3-female	225	501	survived
4-male	200	501	survived
5-female	205	501	died
6-male	230	631	survived
7-female	230	631	survived
8-male	280	631	survived
9-female	215	631	died
10-male	225	631	died
11-female	200	794	survived
12-male	270	794	survived
13-female	220	794	died
14-male	200	794	died
15-female	220	794	died
16-male	220	1000	died
17-female	200	1000	died
18-male	210	1000	died
19-female	215	1000	died
20-male	225	1000	died

DISCUSSION

The Oral LD₅₀ for male and female rats was placed at 700 milligrams per kilogram with lower and upper limits of 620 to 800 milligrams per kilogram.

The compound was classed as mildly toxic by oral ingestion in male and female rats.

Survival time was one to three days.

Toxic signs included reduced appetite and activity (for one to three days in survivors), increasing weakness, ocular discharge containing blood, collapse, and death.

At autopsy there was hemorrhagic lungs, liver discoloration, and acute gastrointestinal inflammation.

Surviving animals were sacrificed seven days after dosing. The viscera appeared normal by macroscopic examination.

Table I-22. THE ACUTE SKIN ABSORPTION MINIMAL
LETHAL DOSE OF FSN-106 FOR RABBITS

Sample Applied Undiluted

Animal No. & Sex	Weight	Dose	Weight Change	Fate
	Kg.	Mg./Kg.	5 Days Later Kg.	
1-male	2.7	50.1	+0.1	survived
2-female	2.3	79.4	+0.1	survived
3-male	2.2	126.0	0.0	survived
4-female	2.4	200.0	--	died - 16 hr
5-male	2.6	501.0	--	died - 16 hr
6-female	2.5	1000.0	--	died - 1 da
7-male	2.1	2000.0	--	died - 16 hr

DISCUSSION

The Acute Skin Absorption Minimal Lethal Dose for male and female rabbits was found to be greater than 126 milligrams per kilogram and less than 200 milligrams per kilogram.

The compound was classed as highly toxic by skin absorption in male and female rabbits.

Survival time as 16 hours to one day.

Toxic signs included reduced appetite and activity (1-3 days in survivors), rapidly increasing weakness, collapse, and death.

At autopsy there was hemorrhagic lungs, slight liver discoloration, and gastrointestinal inflammation.

Surviving animals were sacrificed 14 days after dosing. The viscera appeared normal by macroscopic examination.

Table I-23. SKIN IRRITATION IN RABBITS AFTER
APPLICATION OF FSN-106

Sample (0.2 milliliter) Applied Undiluted

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-female	0	7	7	7	6	6
2-male	0	7	7	7	6	6
3-female	0	7	7	6	6	6
Average	0.0	7.0	7.0	6.6	6.0	6.0

DISCUSSION

The compound was classed as a corrosive irritant when applied undiluted to intact skin of male and female rabbits.

The average maximum score was 7.0 out of a possible 8 in 24 hrs.

Observations following application --

1-hour	No skin changes; zero readings
24-hours	Moderate to severe erythema (slight eschar formation), moderate to severe edema
48-hours	No change
72-hours	No change
120-hours	Severe erythema (eschar formation), slight edema
168-hours	No change

Note: The scab sloughed off in 10-14 days. There was no injury in depth.

Table I-24. EYE IRRITATION IN RABBITS AFTER APPLICATION OF FSN-106

Sample (0.1 milliliter) Applied Undiluted -- 24 hrs exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-female	67	71	65	48	32	27
2-male	69	73	65	40	30	20
3-female	69	71	67	48	35	25
Average	68.3	71.6	66.3	45.3	32.3	24.0

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 71.6 out of a possible 110 in 24 hours.

Observations following application --

Immediate	Discomfort was moderate with pawing and the eyes closed
10-minutes	Slight corneal dullness, moderate to severe erythema, slight edema, copious discharge
1-hour	Opalescent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema, moderate to severe edema, copious discharge
24-hours	Opalescent areas of corneal cloudiness, iris showed no reaction to light, moderate to severe erythema and edema, copious discharge containing whitish exudate
48-168-hours	Gradual improvement
10 days	Barely perceptible corneal cloudiness remained in two instances
14-days	Eyes normal; zero readings

Table I-25. EYE IRRITATION IN RABBITS AFTER
APPLICATION OF FSN-106

Sample (0.1 milliliter) Applied Undiluted -- 15 min exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-female	54	66	54	54	24	10
2-male	73	68	35	31	12	0
3-female	61	69	43	39	15	0
Average	62.6	67.6	44.0	41.3	17.0	3.3

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 67.6 out of a possible 110 in 24 hours.

Observations following application --

Immediate	Discomfort was moderate with pawing and the eyes tightly closed
10-minutes	Slight corneal dullness, moderate to severe erythema, slight to moderate edema, copious discharge
1-hour	Opalescent areas of corneal dullness, iris showed no reaction to light, moderate to severe erythema, moderate to severe edema, copious discharge
24-hours	Opalescent areas of corneal dullness, iris showed no reaction to light, moderate to severe erythema and edema, copious discharge containing whitish exudate
48-120-hours	Gradual improvement
168-hours	Barely perceptible areas of corneal cloudiness in one instance
10-days	Eyes normal; zero readings

Table I-26. THE ORAL LC₅₀ OF MFSN-27 FOR RATS

Sample Fed Undiluted

<u>Animal No. & Sex</u>	<u>Weight Gram</u>	<u>Dose Mg./Kg.</u>	<u>Fate</u>
1-female	210	200	survived
2-male	210	200	survived
3-female	200	200	survived
4-male	220	200	survived
5-female	205	200	survived
6-male	235	251	died
7-female	210	251	survived
8-male	220	251	survived
9-female	210	251	died
10-male	235	251	survived
11-female	210	316	died
12-male	220	316	survived
13-female	200	316	died
14-male	200	316	survived
15-female	210	316	died
16-male	215	398	survived
17-female	200	398	died
18-male	215	398	survived
19-female	200	398	died
20-male	205	398	died
21-female	210	501	died
22-male	240	501	died
23-female	220	501	died
24-male	220	501	died
25-female	235	501	died

DISCUSSION

The Oral LD₅₀ for male and female rats was placed at 310 milligrams per kilogram with lower and upper limits of 270 to 350 milligrams per kilogram.

The compound was classed as moderately toxic by oral ingestion in male and female rats.

Survival time was several hours to five days with most deaths occurring within one day.

Toxic signs included reduced appetite and activity and lethargy (1-4 days in survivors), increasing weakness, collapse, and death.

At autopsy there was lung and liver hyperemia and acute gastrointestinal inflammation.

Surviving animals were sacrificed seven days after dosing. The viscera appeared normal by macroscopic examination.

Table I-27. THE ACUTE SKIN ABSORPTION MINIMAL LETHAL DOSE OF MFSN-27 FOR RABBITS

Sample Applied Undiluted

<u>Animal No. & Sex</u>	<u>Weight Kg.</u>	<u>Dose Mg./Kg.</u>	<u>Animal Weight 5 Days Later Kg.</u>	<u>Fate</u>
1-male	1.9	1000	0.0	survived
2-female	2.2	2000	-0.2	survived
3-male	2.6	3160	-0.1	survived
4-female	2.6	5010	--	died - 4 da
5-male	2.1	7940	--	died - 1 hr
6-female	2.0	7940	--	died - 10 hr
7-male	1.8	7940	--	died - 16 hr

DISCUSSION

The Acute Skin Absorption Minimal Lethal Dose for male and female rabbits was found to be greater than 3160 milligrams per kilogram and less than 7940 milligrams per kilogram.

The compound was classed as slightly toxic by skin absorption in male and female rabbits.

Survival time was one hours to four days.

Toxic signs included reduced appetite and activity and slight lethargy (1-4 days in survivors), increasing weakness, collapse, and death.

At autopsy there was hemorrhagic lungs, liver discoloration, enlarged gall bladder, and gastrointestinal inflammation.

Surviving animals were sacrificed 14 days after dosing. The viscera appeared normal by macroscopic examination.

Table I-28. SKIN IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-27

Sample (0.5 milliliter) Applied Undiluted

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	1	5	5	5	4	1
2-female	1	6	6	6	3	0
3-male	1	5	5	4	3	0
Average	1.0	5.3	5.3	5.0	3.3	0.3

DISCUSSION

The compound was classed as a severe irritant when applied undiluted to intact skin of male and female rabbits.

The average maximum score was 5.3 out of a possible 8 in 24 hrs.

Observations following application --

1-hour	Very slight erythema; no edema
24-hours	Slight to moderate erythema, moderate edema
48-hours	Slight to moderate erythema, moderate edema
72-hours	Slight to moderate erythema and edema
120-hours	Very slight erythema, slight to moderate edema
168-hours	No erythema; very slight edema in one instance

Note: Sample had a defatting effect on the skin causing the skin to flake off in 7-10 days. There was no injury in depth.

Table I-29. EYE IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-27

Sample (0.1 milliliter) Applied Undiluted -- 24 hr exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	16	51	51	51	27	17
2-female	18	75	89	89	49	32
3-male	18	75	73	73	47	32
Average	17.3	67.0	71.0	71.0	41.0	27.0

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 71.0 out of a possible 110 in 48 hours.

Observations following application -- 24 hours exposure

Immediate	Discomfort was severe, with pawing, squealing, and the eyes closed
10-minutes	Moderate erythema and edema, copious discharge
1-hour	Moderate erythema, moderate to severe edema, copious discharge
24-hours	Opalescent areas of corneal cloudiness, iris showed little or no reaction to light, moderate to severe erythema and edema, copious discharge containing whitish exudate
48-hours	Opalescent to opaque areas of corneal cloudiness, iris showed little or no reaction to light, moderate to severe erythema, moderate edema, copious discharge containing whitish exudate
72-120-hours	Slight improvement
168-hours	Diffuse to easily discernible areas of corneal cloudiness, moderate erythema, slight edema, moderate discharge
10-14-days	Gradual improvement
17-days	Two were scored zero
20-days	Eyes normal; zero readings

Table I-30. EYE IRRITATION IN RABBITS AFTER
APPLICATION OF MFSN-27

Sample (0.1 milliliter) Applied Undiluted -- 15 min exposure

Animal No. & Sex	Numerical Evaluation at the End of (hr)					
	1	24	48	72	120	168
1-male	16	61	57	57	57	47
2-female	16	53	61	45	35	35
3-male	16	63	67	47	35	33
Average	16.0	62.3	58.3	49.6	42.3	38.3

DISCUSSION

The compound was classed as a severe eye irritant in male and female rabbits. The average maximum score was 62.3 out of a possible 110 in 24 hours.

Observations following application -- 15 minutes exposure

Immediate	Discomfort was severe with pawing, squealing, and the eyes tightly closed
10-minutes	Moderate erythema and edema, copious discharge
1-hour	Moderate erythema and edema, copious discharge
24-hours	Translucent to opalescent areas of corneal cloudiness, iris reaction to light was sluggish, moderate to severe erythema, moderate edema, copious discharge containing whitish exudate
48-120-hours	Slight improvement
168-hours	Slight areas of translucent corneal cloudiness, iris reaction to light was sluggish, moderate erythema, very slight to slight edema, slight to moderate discharge
10-17-days	Gradual improvement
20-days	Slight areas of translucent corneal cloudiness in one instance; two scored zero

APPENDIX J

MONSANTO RUB-BLOCK LUBRICATION/WEAR TEST MACHINE

This machine was designed and built by Monsanto Company to test various lubricating fluid systems in sliding frictional contacts under a wide range of temperatures and pressures. It consists essentially of a vertical spindle fitted with a testing disk (ring) immersed in a thermostatted reservoir of the test fluid. Two test blocks are radially loaded against the ring and are restrained from rotating about the ring axis by a torque pickup. The blocks may be either flat or conforming. Mechanical details are shown in Figure J-1. An overall view of the machine and its auxiliaries appears in Figure J-2.

Friction coefficients are determined by torque transfer measurements from the rotating cylindrical ring to stationary wear blocks. Wear measurements are obtained by analysis of photographs of the wear tracks on non-conforming test blocks. Wear block temperature is determined by embedded thermocouples.

The loading systems, torque measurements systems, and wear specimens are contained in a closed chamber where controlled temperature and pressure are maintained. For liquid lubricant studies the wear specimens are submerged while bonded lubricant studies are carried out in a dry system. The rotating shaft passes through a mechanical shaft seal and is externally driven by a variable speed motor and belt arrangement. Reciprocating motion of the ring with variable angular displacement is accomplished by a four bar linkage.

Range of Operating Conditions

The operating range specifications of the Monsanto Friction and Wear Machine are listed below:

Radial Block Load: 2 to 1600 lb_f; continuously variable from outside the test chamber.

Rotational Motion: 100 to 3390 rpm from 5 HP motor with capability of 10,000 rpm with suitable pulleys.

Reciprocating Drive: 0 to 45° angular displacement with frequencies to 3000 cpm.

Wear Specimen Geometry: Conforming or flat wear block on 1.5 in. diameter ring (std). Other geometries are available.

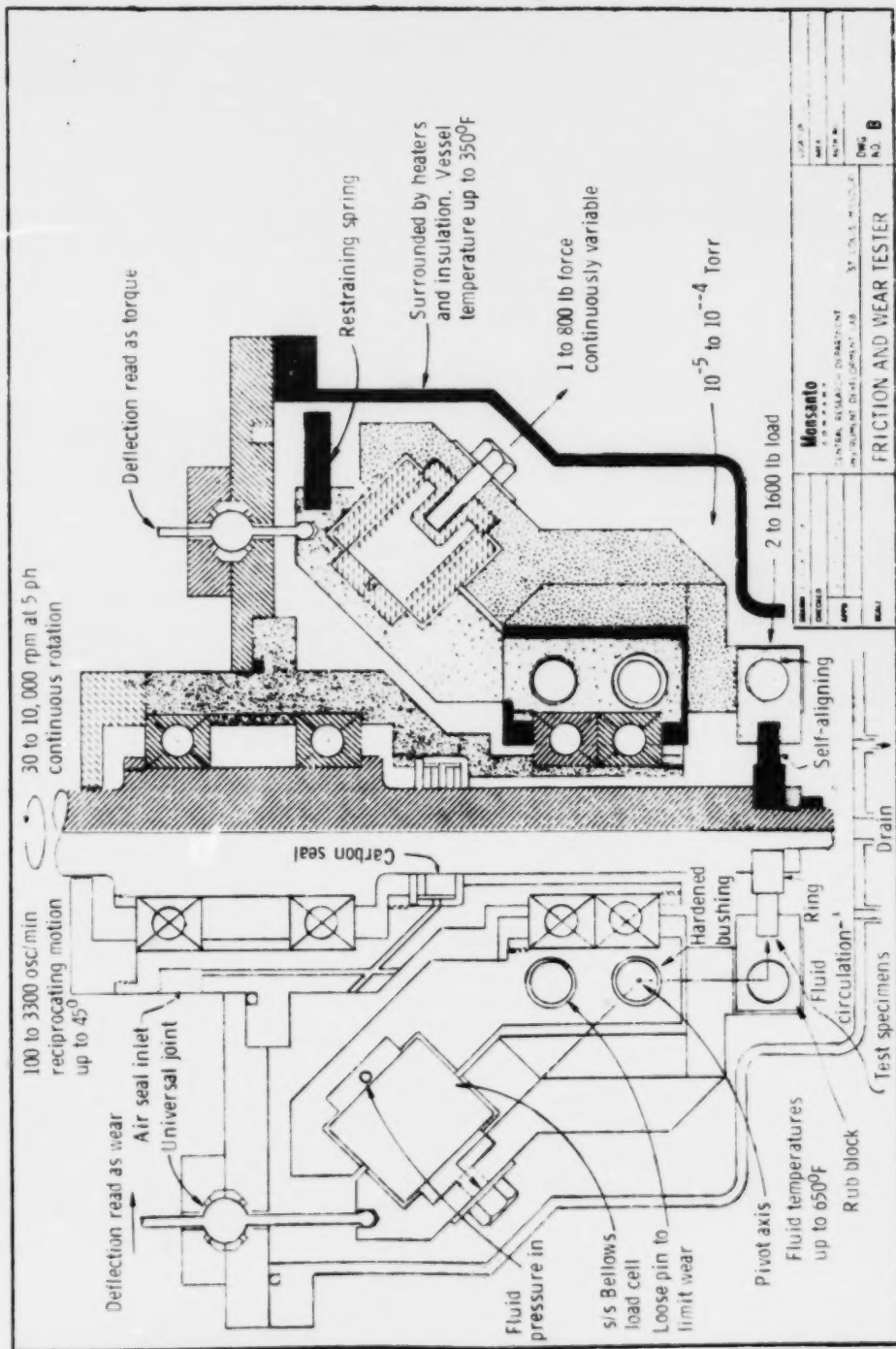
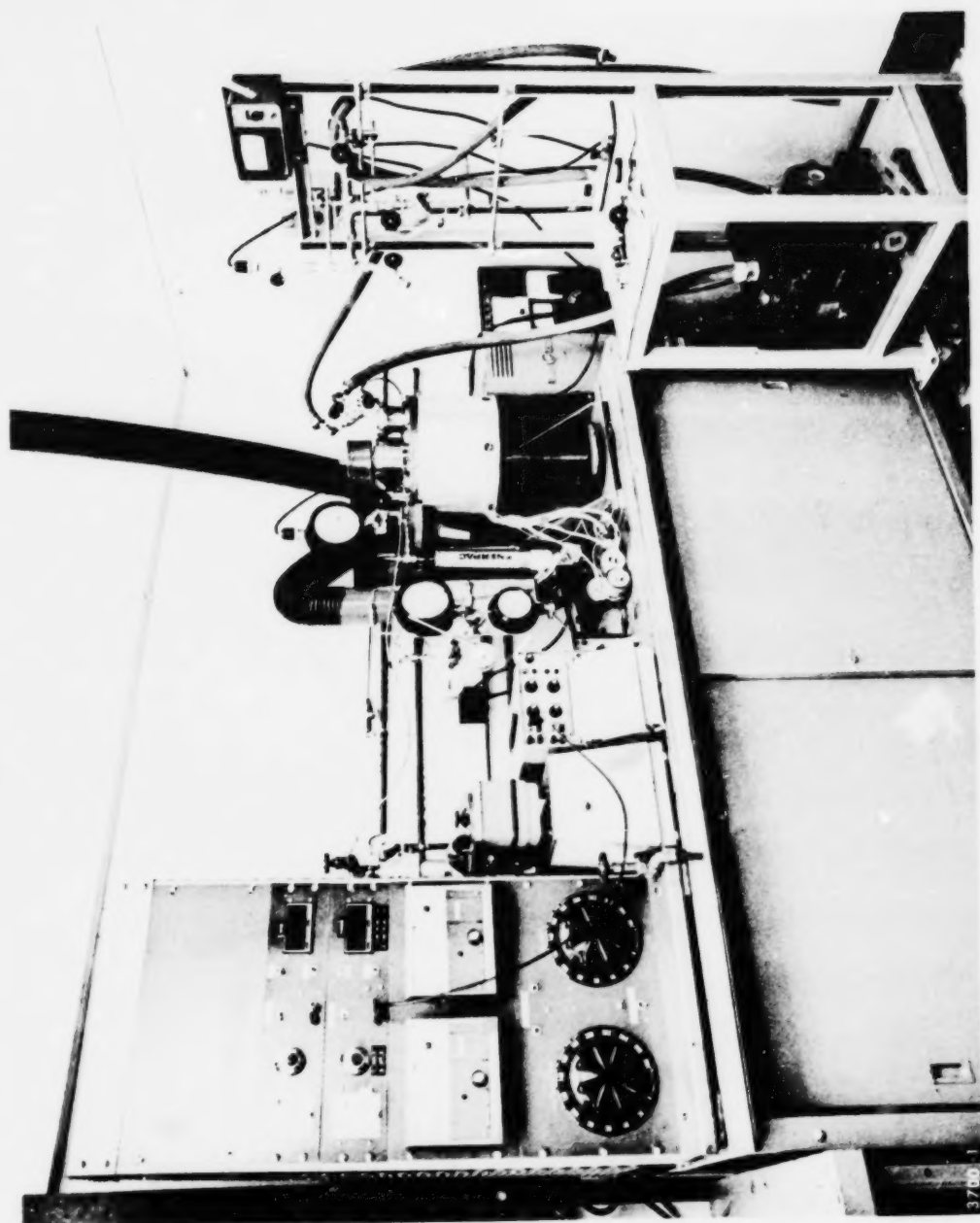


Figure J-1. Rub Block Lubrication/Wear Test Machine



J-3. TEST SETUP

Lubricant Temperature: Room to 650°F.

Pressure: Chamber pressure range is from 10^{-5} to 10^4 Torr.

Data Available: Friction torque and wear depth are continuously available during operation. Wear specimens are available for examination and photography at end of run.

Liquid Lubricant Operating Procedure:

- (1) Wear block and ring metallurgy, surface roughness and geometry are specified.
- (2) Range of operating condition simulative of the end use machine is chosen.
- (3) Strain gauge instrumentation, pressure transducers and thermocouples are calibrated.
- (4) Lubricant is placed in the closed chamber and the desired temperature and pressure are equilibrated.
- (5) (a) For conforming geometries a break-in procedure which allows repeatable friction coefficients under given load and speeds is determined. The speed is then fixed at the lowest value specified and the load is increased in increments until an incipient scuffing torque measurement is observed. The speed is increased and the loading procedure repeated until the maximum specified speed is reached.

(b) For flat block or low conforming geometries the load and speed are fixed with the friction and wear observed for a fixed time or until excessive wear occurs. New test specimens are used for each load and speed combination.

Significance

Wear and friction are determined as a function of speed, load, and temperature for each fluid formulation, metallurgy, wear specimen shape. Hydrodynamic, mixed, and boundary lubrication regimes are investigated under loads, speeds, and environments seen in real bearings.

APPENDIX K

THERMODYNAMIC PROPERTIES OF MULTICOMPONENT FLUIDS Computer Program E1393

1. SCOPE

Computer program E1393 computes the density, enthalpy, and entropy of multicomponent fluids in the subcooled liquid, saturated liquid, saturated vapor, and superheated vapor regions. Output tables contain:

- (a) Bubble point pressures and saturated liquid properties at specified temperature intervals.
- (b) Dew point pressures and saturated vapor properties at specified temperature intervals.
- (c) Bubble point temperatures and saturated liquid properties at specified pressures.
- (d) Dew point temperatures and saturated vapor properties at specified pressures.
- (e) Single phase liquid and vapor properties at specified pressures and specified temperature intervals.

2. MODEL

Saturation conditions are described by the Antoine equation for vapor pressure, the van Laar equation for liquid phase non-idealities, the Redlich-Kwong equation of state for gas volume, and the Poynting equation for liquid phase fugacity. Liquid density is described by Benson's correlation (Ref. 1, p 77) and the temperature dependence of the latent heat of vaporization is given by the Watson equation (Ref. 1, p 148).

A Fortran source listing of the models is given in Section 7. The main program reads the input data and calls subroutines MODEL and OUTPUT. Subroutine MODEL controls the generation of the physical property tables which are subsequently printed by subroutine OUTPUT.

The individual property calculations are made in modular subprograms whose entry point names and functions are given below.

<u>Entry</u>	<u>Function</u>
KAI	To compute the component vapor-liquid distribution ratios.
SAT	To control subprograms which compute the bubble liquid and dew gas properties at a specified temperature.
SPGC	To compute the gas fugacity of a component at T, P.
PSAMVL	To compute the liquid phase activity coefficients of all components.
SHGC	To compute the gas enthalpy of a component at T, P.
SHGM	To compute the gas enthalpy of a mixture at T, P.
SHLB	To compute the bubble liquid enthalpy at T.
SHLL	To compute the liquid enthalpy at T and P.
SHVC	To compute the latent heat of vaporization of a pure component at T.
SPSC	To compute the vapor pressure of a pure component at T.
SSGC	To compute the gas entropy of a pure component at T, P. This entry point was used in the final program.
SSGM	To compute the gas entropy of a mixture at T, P.
SSLB	To compute the bubble liquid entropy at T.
SSLL	To compute the liquid entropy at T, P.
STB	To invoke subprograms which compute the bubble liquid temperature, volume, enthalpy, and entropy at P.
STD	To invoke subprograms which compute the dew gas temperature, volume, enthalpy, and entropy at P.
SVGC	To compute the gas volume of pure component at T, P.
SVGM	To compute the gas volume of a mixture at T, P.
SVLC	To compute the liquid volume of a pure component at T.
SVLM	To compute the liquid volume of a mixture at T.

The library routines used by Program E1393 are described in Section 8.

3. INPUT

Problem data is entered on Input Data Sheets as shown in Section 9. Blank forms are provided in Section 11. The input comprises 11 lists as follows:

- List 1: Problem title (printed on each output page)
- List 2: Problem subtitle (printed on each output page)
- List 3: Temperature grid limits and spacing
- List 4: Pressure grid points
- List 5: System composition in mole or mass units
- List 6: Component names, molecular weights, and Antoine vapor pressure equation constants
- List 7: Liquid activity coefficient data for van Laar A_{ij}
- List 8: Liquid activity coefficient data for van Laar C_{ij}
- List 9: Temperature coefficients for the ideal gas heat capacity of the components
- List 10: Component critical properties, heat of vaporization, and liquid density
- List 99: End of case indicator

Lists 2, 7, and 8 may be omitted. If List 7 and 8 are not used, the program assumes that the liquid is an ideal solution.

Data is key punched onto cards as indicated on the Input Data Sheets. Numeric items must be separated by one or more blanks. A list may be freely continued onto additional cards but a data item must not straddle card boundaries.

4. OUTPUT

The program results are the tables described in Paragraph 1. Section 10 gives an example corresponding to the input data in Section 9. The column headings are self-explanatory.

5. EXECUTION

The program was compiled on an IBM 370/165 computer with the Fortran IV G Level 20 compiler. Compiled subprograms were combined with library routines by IBM's F88 Level Linkage Editor and the resulting load module was saved for production runs. The program requires 130K bytes of core where 1K = 1024.

6. REFERENCES

- (1) Reid, R. C., and T. K. Sherwood, "The Properties of Gases and Liquids," McGraw-Hill (1966).

7. FORTTRAN SOURCE LISTING OF PROGRAMS DEVELOPED FOR E1393

```

C      PROGRAM E1393 - THERMODYNAMIC PROPERTIES OF FLUID MIXTURES
C IDENTIFICATION SECTION
C      TITLE      = THERMODYNAMIC PROPERTIES OF FLUID MIXTURES
C      AUTHOR     = A C PAULS
C      LOCATION   = CED, MONSANTO CO., ST. LOUIS, MO.
C      DATE       = 9/71, 2/72
C      FILES      = FORTRAN 5, 6, 12
C      SUBPROGRAMS = KAI1, MAIN, MODEL, OUTPUT, SAT1, SFG1, SGAMV1,
C                  SHG1, SHL1, SHV1, SPS1, SSG1, SSL1, STAL, STD1,
C                  SVG1, SVL1
C      LIBPROGRAMS = DATE4, HEADER, KTBL, LINE, MASS, MOVE, MPBPP,
C                  MPBPT, NCK, NORM, ROOTFD, UCP, UCT, ZERO, ZRKC
C
C DEFINITION SECTION
C      AA(I,K)    ANTOINE VAPOR PRESSURE DATA FOR COMPONENT I
C      AM         REDLICH-KWONG CONSTANT FOR MIXTURE
C      ARK(I)     REDLICH-KWONG CONSTANT FOR COMPONENT I
C      RM         REDLICH-KWONG CONSTANT FOR MIXTURE
C      RHK(I)     REDLICH-KWONG CONSTANT FOR COMPONENT I
C      C(I,K)     IDEAL GAS HEAT CAPACITY CONSTANTS FOR COMPONENT I
C      D          DENSITY, LB/FT3
C      DB(I)      INPUT DATA BASE
C      DLG(I)     DERIVATIVE OF LN GAM(I) WITH RESPECT TO T
C      DL1(I)     LIQUID DENSITY OF COMPONENT I AT DB(I+420), GMOL/CM3
C      FG(I)      GAS FUGACITY OF COMPONENT I AT SYSTEM PRESSURE, ATM
C      FL(I)      LIQUID FUGACITY OF COMPONENT I AT SYSTEM PRESSURE, ATM
C      FLG(I)     IDEAL SOLUTION K-VALUE FL(I)/FG(I)
C      GA(I,J,K)  LIQUID ACTIVITY COEFFICIENT DATA FOR AIJ
C      GAM(I)     LIQUID ACTIVITY COEFFICIENT OF COMPONENT I
C      GK(I,J,K)  LIQUID ACTIVITY COEFFICIENT DATA FOR CIJ
C      HB        BUBBLE POINT LIQUID ENTHALPY, CAL/GMOL
C      HD        DEW POINT GAS ENTHALPY, CAL/GMOL
C      HG        GAS ENTHALPY, CAL/GMOL
C      HL        LIQUID ENTHALPY, CAL/GMOL
C      HZ        LIQUID ENTHALPY AT 0 DEG C AND BUBBLE POINT PRESSURE
C      ICC       INPUT COMPOSITION UNIT: 1 = MASS, 2 = MOLE
C      KERR       ERROR CODE: 1 = NO, 2 = YES
C      KGAM      LIQUID ACTIVITY COEFFICIENT EQUATION: 1 = VAN LAAR
C      KUP        PRESSURE UNIT: 1 = ATM, 2 = PSI, 3 = MMHG
C      KUT        TEMPERATURE UNIT: 1 = C, 2 = F, 3 = K, 4 = R
C      NAME(L,I)  NAME OF COMPONENT I
C      NC        NUMBER OF COMPONENTS
C      NLC       NUMBER OF COMPONENTS
C      NP        NUMBER OF ISOBARS
C      NT        NUMBER OF ISOTHERMS
C      P         PRESSURE, ATM
C      PH        BUBBLE POINT PRESSURE, ATM
C      PC(I)     CRITICAL PRESSURE OF COMPONENT I, ATM
C      PCM       CRITICAL PRESSURE OF MIXTURE, ATM
C      PD        DEW POINT PRESSURE, ATM
C      PG(I)     GRID PRESSURE FOR I-TH ISOBAR, ATM
C      R         GAS CONSTANT, ATM-CM3/GMOL-K
C      RE(I,J)   SATURATION PROPERTIES FOR I-TH ISOTHERM
C      RG(I,J,K) PROPERTIES AT ISOTHERM I & ISOBAR J
C      RM        GAS CONSTANT, CAL/GMOL-K
C      SH        BUBBLE POINT LIQUID ENTROPY, CAL/GMOL-K
C      SD        DEW POINT GAS ENTROPY, CAL/GMOL-K

```



```

C      SG      GAS ENTROPY, CAL/GMOL-K
C      SL      LIQUID ENTROPY, CAL/GMOL-K
C      SZ      LIQUID ENTROPY AT 0 DEG C AND BUBBLE POINT PRESSURE
C      T      TEMPERATURE, DEG K
C      TC(I)   CRITICAL TEMPERATURE OF COMPONENT I, DEG K
C      TCM     CRITICAL TEMPERATURE OF MIXTURE, DEG K
C      TG(I)   GRID TEMPERATURE FOR I-TH ISOTHERM, DEG K
C      TLL     TEMPERATURE GRID LOWER LIMIT
C      TLU     TEMPERATURE GRID UPPER LIMIT
C      TSS     TEMPERATURE GRID STEP SIZE
C      VB      BUBBLE POINT LIQUID VOLUME, CM3/GMOL
C      VCM     CRITICAL VOLUME OF MIXTURE, CM3/GMOL
C      VD      DEW POINT VOLUME, CM3/GMOL
C      VG      GAS VOLUME, CM3/GMOL
C      WM(I)   MOLECULAR WEIGHT OF COMPONENT I, G/GMOL
C      WMM     MOLECULAR WEIGHT OF MIXTURE, LB/LBMOL
C      X(I)    MASS FRACTION OF COMPONENT I IN SYSTEM
C      Z(I)    MOLE FRACTION OF COMPONENT I IN SYSTEM
C      PROGRAM E1393
C DECLARATIVE SECTION
COMMON      DB(1600), GA(20,20,3), GK(20,20,3)
COMMON/LITD/ NAME(3,20)
COMMON /TITL/ DATE(2), TTL1(15), TTL2(15)

C
C FILE SECTION
900 FORMAT(G1.0)
901 FORMAT( 3A4, (G1.0) )
902 FORMAT(3X, 15A4)

C
C INPUT SECTION
C      INITIALIZE CONTROL SUBROUTINE + PROG NO.
C      CALL DATE4(DATE)
C      CALL HEADER(-1393)
C      READ LIST NUMBER, CONTROL LISTS
5 READ (5, 900, END = 8) LN
GO TO (11, 12, 13, 14, 15, 16, 17, 18, 19, 20), LN
IF (LN .EQ. 99) GO TO 30
+ CONTINUE
CALL EXIT
C      INITIALIZE PROBLEM-SET
11 CALL ZERO(DB, 1, 4000)
READ (12, 902) TTL1
GO TO 5
C      LIST 2, CASE TITLE
12 READ (12, 902) TTL2
GO TO 5
C      LIST 3, TEMPERATURE GRID
13 READ (5, 900) (DB(I), I=2,6)
GO TO 5
C      LIST 4, PRESSURE GRID
14 READ (5, 900) DB(12), N, (DB(I + 50), I = 1, N)
DB(13) = N
GO TO 5
C      LIST 5, SYSTEM COMPOSITION
15 READ (5, 900) DB(19), N, (DB(I+100), I=1,N)
DB(20) = N
GO TO 5
C      LIST 6, MOLECULAR WEIGHTS AND ANTHINE

```



```

C          CONSTANTS
16 READ (5,900) N
   DB(21) = N
   DO 160 I = 1,N
160 READ (5,901) (NAME(J,I), J=1,3), DB(I+120), DB(I+140),
   DB(I+160), DB(I+180)
   GO TO 5
C          LIST 7, LIQ. ACT. COEF. DATA FOR A(I,J)
17 READ (5,900) N, DB(23), (I, J, (GA(I,J,K), K=1,3),
   (GA(J,I,K), K=1,3), I=1,N)
   DB(22) = N
   GO TO 5
C          LIST 8, LIQ. ACT. COEF. DATA FOR C(I,J)
18 READ (5,900) N, DB(25), (I, J, (GK(MIN0(I,J), MAX0(I,J), K),
   K=1,3), I=1,N)
   DB(24) = N
   GO TO 5
C          LIST 9, IDEAL GAS HEAT CAPACITY CONSTANTS
19 READ (5,900) N, ((DB(I + J*20 + 180), J=1,4), I=1,N)
   DB(26) = N
   GO TO 5
C          LIST 10, CRITICAL PROPERTIES, HEAT OF
C          VAPORIZATION, LIQUID DENSITY
20 READ (5,900) N, ((DB(I + 20*J + 300), J=1,6), I = 1,N)
   DB(27) = N
   GO TO 5
C          SOLVE MODEL
30 CALL MODEL
C          PRINT CASE RESULTS
C          CALL OUTPUT
   GO TO 5
END

```

BLOCK DATA
COMMON /TITL/ DATE(2), TTL(30)
DATA TTL/30*4H /
END

```

SUBROUTINE MODEL
C
C DEFINITION SECTION
C
C DECLARATIVE SECTION
COMMON DB(120), WM(20), AA(20,3), C(20,6),
1 TC(20), PC(20), Z361(140),
2 AM, BM, Z503(78),
3 ARK(20), BRK(20), DLG(20), DL1(20), FG(20), FL(20),
4 FLG(20), GAM(20), G1(20), G2(20), Z(20),
5 TG(50), PG(50), RE(50,8), Z1301(300),
6 GA(20,20,3), GK(20,20,3), RG(50,50,3)
COMMON /COM1/ KEHR(2), KUP, KUT, NC, NP, NT, PCM, HZ, SZ
COMMON/CONTRL/ NLC, KDUM(3)
DATA R/82.0575/, RH/1.9872/
C
C COMPUTATION SECTION
ZERO OUTPUT END OF DATA BASE
C
CALL ZERO(DB, 501, 1600)
CALL ZERO (RG, 1, 7500)
C
KUT = DB(2) + 1
TLL = DB(3)
TLU = DB(4)
TSS = DB(5)
KUP = DB(12) + 1
NP = DB(13)
ICC = DB(19)
NC = DB(20)
NLC = NC
KGAM = DB(23)
C
C SYSTEM COMPOSITION IN MOLE FRACTION
C LIQUID DENSITY, GMOL/CM3
C
SUM = 0.
DO 10 I = 1, NC
Z(I) = DB(I + 100)
DL1(I) = DB(I + 400)/WM(I)
IF (ICC .EQ. 1) Z(I) = Z(I)/WM(I)
10 SUM = SUM + Z(I)
DO 12 I = 1, NC
Z(I) = Z(I)/SUM
12 GAM(I) = 1.0
C
C INITIALIZE SUBPROGRAM PARAMETERS
C
I = KAI1(FG, FL, FLG, GAM, KGAM, NC, PC, H, TC, WM)
CALL SGAMV1 (GA, GAM, GK, NC)
C
CALL SPS1 (AA)
CALL SVG1 (NC, Z, TC, PC, R, ARK, BRK, AM, BM)
PCM = (R*(0.0866403/BM)**5*(AM/0.427480)**2)**0.33333333
TCM = (0.0866403*AM/(0.427480*BM*R))**0.66666667
VCM = R*TCM/(3*PCM)
CALL SHV1 (NC, DB(361), DB(381), TC, TCM)
CALL SHG1 (NC, Z, C, ARK, BRK, AM, BM, H, RH)
CALL SSG1 (NC, Z, C, 273.15, 1.0, ARK, BRK, AM, BM, R, RH)
CALL SFG1 (ARK, BRK, R)

```

```

CALL SVL1 (NC, Z, DL1, UB(421), TC, PC, R, TCM, PCM)
CALL SHL1 (NC, Z, R, RH, TC)
CALL SSL1 (NC, Z, R, RH, TC)
CALL SAT1(Z, NC, TCM, PCM, VCM, GAM, KERR, KGAM)
CALL STB1(Z, NC, TCM, PCM, VCM, GAM, KERR, KGAM)
CALL STD1(Z, NC, TCM, PCM, VCM, GAM, KERR, KGAM)

C
C          SETUP GRID POINTS IN DEG K, ATM
DO 16 I      NT = AMIN1(2 + (TLU - TLL)/TSS, 50.0)
16          TG(I) = TLL + (I - 2)*TSS
CALL UCT (NT, KUT, 3, TG, TG)
          TG(1) = 273.15
CALL UCP (NP, KUP, 1, DB(5), PG)

C
C          SCAN TEMPERATURE GRID
          PD = 0.
          HZ = 0.0
          SZ = 0.0
DO 70 I      = 1, NT
C          SATURATION PROPERTIES AT T
          T = TG(I)
          IF (T .GT. TCM) GO TO 60
CALL SAT(T, PD, VD, HD, SD, PB, VB, HB, SB)
          IF (KERR(1) .NE. 1) WRITE (6,941) T, PB
          IF (KERR(2) .NE. 1) WRITE (6,942) T, PD
941 FORMAT(// ' BUBBLE POINT ERROR. T, PB = ', 2G13.5)
942 FORMAT(// ' DEW POINT ERROR. T, PD = ', 2G13.5)

C
          IF (I .EQ. 1) HZ = HB
          IF (I .EQ. 1) SZ = SB
          RE(I,1) = PB
          RE(I,2) = VB
          RE(I,3) = HB - HZ
          RE(I,4) = SB - SZ
          RE(I,5) = PD
          RE(I,6) = VD
          RE(I,7) = HD - HZ
          RE(I,8) = SD - SZ

C
C          V, H, S AT GRID PRESSURES
60 DO 65 J      = 1, NP
          P = PG(J)
          IF (T .GT. TCM) GO TO 61
          IF (P .GT. PD) GO TO 62
61 CALL SVGM (T, P, VG)
CALL SHGM (T, P, VG, HG)
CALL SSGM (T, P, VG, SG)
          RG(I,J,1) = VG
          RG(I,J,2) = HG - HZ
          RG(I,J,3) = SG - SZ
          GO TO 65
62 IF (P .LT. PB) GO TO 65
CALL SHLL (T, P, PB, HB, HL)
CALL SSLL (T, P, PB, SB, SL)
          RG(I,J,1) = VB
          RG(I,J,2) = HL - HZ
          RG(I,J,3) = SL - SZ

```

65 CONTINUE
70 CONTINUE
RETURN
END

```

SUBROUTINE OUTPUT
COMMON      DB(780), Z(20), TG(50), PG(50), RE(50,8),
1           Z1301(2700), RG(50,50,3)
COMMON/LITD/ NAME(3,20)
COMMON /COM1/ KEHR(2), KUF, KUT, NC, NP, NT, PCM, HZ, SZ
REAL WM(20), X(20)
INTEGER*2   LT(4)/2H C, 2H F, 2H K, 2H R/
DIMENSION   ZP(20)
EQUIVALENCE (DB(121), WM(1))
920 FORMAT( '0', 'COMPOSITION', 8X, 'MOLE %', 10H      MASS %,
1           10H      MOLE WT)
924 FORMAT( ' ', 13, 1X, 3A4, F9.3, F10.3, F10.2)
928 FORMAT( ' ', 4X, 'MIXTURE', 7X, '100.000', 10H      100.000, F10.2)
930 FORMAT(///)
932 FORMAT( '0', 'THERMODYNAMIC PROPERTIES AT SATURATION')
936 FORMAT( ' ', 3X, 'TEMP', 9X, '----- BUBBLE POINT LIQUID'
1           , '-----')
3           / ' ', 5X, 'T', 10X, 'P', 14X, 'D', 14X, 'H', 14X, 'S'
5           / ' ', 3X, 'DEG', A2, 7X, 'PSI', 10X, ' LB/FT3', 7X,
6           ' BTU/LB', 6X, ' BTU/LB-F ', 2X)
938 FORMAT( ' ', 3X, 'TEMP', 9X, '----- DEW POINT GAS --'
1           , '-----')
3           / ' ', 5X, 'T', 10X, 'P', 14X, 'D', 14X, 'H', 14X, 'S'
5           / ' ', 3X, 'DEG', A2, 7X, 'PSI', 10X, ' LB/FT3', 7X,
6           ' BTU/LB', 6X, ' BTU/LB-F ', 2X)
940 FORMAT( ' ', F8.2, F12.2, 4X, 3G15.4, F11.2, 4X, 3G15.4)
944 FORMAT( '0', 'THERMODYNAMIC PROPERTIES IN SINGLE PHASE REGION')
948 FORMAT( ' ', 3X, 'TEMP'
1           / ' ', 5X, 'T', 11X, 'P', 8X, 'D', 14X, 'H', 14X, 'S'
2           / ' ', 3X, 'DEG', A2, 8X, 'PSI', 4X, ' LB/FT3', 7X,
3           ' BTU/LB', 6X, ' BTU/LB-F ')
952 FORMAT( ' ', F8.2, F11.2, 3G15.4)

```

C
C

CONVERT TO ENGLISH UNITS

```

CALL UCT(NT, 3, KUT, TG, TG)
CALL UCP(NP, 1, 2, PG, PG)
CALL UCP(NT, 1, 2, RE(1,1), RE(1,1))
CALL UCP(NT, 1, 2, RE(1,5), RE(1,5))
CALL MASS(NC, WM, Z, ZS, X, XS, WMM)
CALL NORM(NC, X, XS, X)
DO 15 I = 1, NT
  RE(I,2) = RE(I,2)/WMM*0.0160185
  RE(I,3) = RE(I,3)/WMM*1.8
  RE(I,4) = RE(I,4)/WMM
  RE(I,6) = RE(I,6)/WMM*0.0160185
  RE(I,7) = RE(I,7)/WMM*1.8
  RE(I,8) = RE(I,8)/WMM
  IF (RE(I,2) .NE. 0.0) RE(I,2) = 1.0/RE(I,2)
  IF (RE(I,6) .NE. 0.0) RE(I,6) = 1.0/RE(I,6)
DO 15 J = 1, NP
  RG(I,J,1) = RG(I,J,1)/WMM*0.0160185
  IF (RG(I,J,1) .NE. 0.0) RG(I,J,1) = 1.0/RG(I,J,1)
  RG(I,J,2) = RG(I,J,2)/WMM*1.8
15  RG(I,J,3) = RG(I,J,3)/WMM
DO 10 I = 1, NC
  X(I) = 100.0*X(I)
10  ZP(I) = 100.0*Z(I)

```


C
C
C

SATURATION TEMPERATURE TABLE

```
CALL HEADER(1)
WRITE (6,920)
DO 22 I = 1, NC
22 WRITE (6,924) I, (NAME(J,I), J=1,3), ZP(I), X(I), WM(I)
WRITE (6,928) WM
IDUM = LINE(3*NC)
CALL KTBL(2, 3, 5)
WRITE (6,932)
```

C

BUBBLE POINT LIQUID

```
WRITE (6,936) LT(KUT)
DO 24 I = 2, NT
IF (RE(I,1) .EQ. 0.0) GO TO 26
IF (KTBL1(KODE) .EQ. 1) WRITE(6,936) LT(KUT)
24 WRITE (6,940) TG(I), (RE(I,J), J=1,4)
26 WRITE (6,930)
```

C

DEW POINT GAS

```
CALL KTBL(4, 3, 5)
WRITE (6,938) LT(KUT)
DO 28 I = 2, NT
IF (RE(I,1) .EQ. 0.0) GO TO 30
IF (KTBL1(KODE) .EQ. 1) WRITE(6,938) LT(KUT)
28 WRITE (6,940) TG(I), (RE(I,J), J=5,8)
```

C
C

SATURATION PRESSURE TABLE

```
30 CALL HEADER(1)
CALL KTBL(2, 3, 5)
WRITE (6,932)
```

C

BUBBLE POINT LIQUID

```
WRITE (6,936) LT(KUT)
TK = 273.15
DO 45 I = 1, NP
P = PG(I)/14.696
IF (P .GT. PCM) GO TO 50
CALL STB (TK, P, V, H, S)
CALL UCT(1, 3, KUT, TK, T)
D = 0.0
IF (V .GT. 0.0) D = WM/(V*0.0160185)
H = (H - HZ)/WM*1.8
S = (S - SZ)/WM
IF (KTBL1(KODE) .EQ. 1) WRITE(6,936) LT(KUT)
45 WRITE (6,940) T, PG(I), D, H, S
```

C
C

DEW POINT GAS

```
50 WRITE (6,930)
CALL KTBL(4, 3, 5)
WRITE (6,938) LT(KUT)
DO 55 I = 1, NP
P = PG(I)/14.696
IF (P .GT. PCM) GO TO 60
CALL STD (TK, P, V, H, S)
CALL UCT(1, 3, KUT, TK, T)
D = 0.0
IF (V .GT. 0.0) D = WM/(V*0.0160185)
H = (H - HZ)/WM*1.8
S = (S - SZ)/WM
```

```

      IF (KTBL1(KODE) .EQ. 1) WRITE(6,938) LT(KUT)
55 WRITE (6,940) T, PG(I), D, H, S

```

```

C
C          SUBCOOLED-SUPERHEATED TABLE

```

```

60 CALL HEADER(1)
   WRITE (6,920)
   DO 62 I = 1,NC
62  WRITE (6,924) I, (NAME(J,I), J=1,3), ZP(I), X(I), WM(I)
   WRITE (6,928) WMM
   IDUM = LINE(3+NC)
   CALL KTBL(2, 3, 5)
   WRITE (6,944)
   WRITE (6,948) LT(KUT)
   DO 64 J = 1,NP
   DO 64 I = 2,NT
   IF (KTBL1(KODE) .EQ. 1) WRITE (6,948) LT(KUT)
64  WRITE (6,952) TG(I), PG(J), (RG(I,J,K), K=1,3)
   RETURN
   END

```

```

C      FUNCTION      KAI1(FG, FL, FLG, GAM, /KGAM/, /NC/, PC, R, TC, WM)
C      TITLE         VAPOR-LIQUID DISTRIBUTION RATIOS
C      SUBPROGRAMS    SFGC, SGAMVL, SPSC, SVLC
C      L              CALL CODE: 1 = FIRST CALL; 2 = T AND P SAME AS
C                      LAST CALL; 3 = XC AND YC SAME AS LAST CALL.
C      XC(I)          MOLE FRACTION OF COMPONENT I IN LIQUID
C      XK(I)          VAPOR-LIQUID DISTRIBUTION RATIO FOR COMPONENT I
C      YC(I)          MOLE FRACTION OF COMPONENT I IN VAPOR
C
C      REAL           FG(1), FL(1), FLG(1), GAM(1), PC(1), TC(1), WM(1),
1      XCS(20)
C      REAL*8         PSIA, TF, XC(1), XK(1), YC(1)
C
C      KAI1 = 1
C      RETURN
C
C      ENTRY          KAI(XK, TF, PSIA, XC, YC, L)
C      P              = PSIA/14.696
C      T              = (TF - 32.)/1.8 + 273.15
C                      FUNCTIONS DEPENDENT ON T AND P
C      IF (L .EQ. 2) GO TO 40
C      DO 38 I = 1, NC
C          CALL SFGC (I, T, P, FG(I))      PURE COMPONENT GAS FUGACITY AT SYSTEM P
C          CALL SVLC (I, T, PS, VL)        PURE COMPONENT LIQUID FUGACITY AT SYSTEM P
C          CALL SPSC (I, T, PS)            FROM VAPOR PRESSURE AND GAS FUGACITY
C          CALL SFGC (I, T, PS, FGS)
C          FL(I) = FGS*EXP(VL*(P - PS)/(R*T))
C                      K-VALUE FOR IDEAL SOLUTIONS
C      38      FLG(I) = FL(I)/FG(I)
C
C                      K-VALUE FOR NON-IDEAL LIQUID SOLUTION
C      40 DO 42 I = 1, NC
C          XK(I) = FLG(I)
C      42      XCS(I) = XC(I)
C          IF (KGAM .EQ. 0) GO TO 50
C          CALL SGAMVL (T, XCS)
C          DO 44 I = 1, NC
C      44      XK(I) = GAM(I)*FLG(I)
C      50      KAI = 1
C      RETURN
C      END

```

```

SUBROUTINE SAT1(Z, NC, TCM, PCM, VCM, GAM, KERR, KGAM)
C
C DEFINITION SECTION
C ALPHA      MOLES OF VAPOR PER MOLE OF FEED
C BETA       MOLES OF LIQUID 1 PER MOLE OF TOTAL LIQUID
C MPBPP      FUNCTION ERROR CODE: 1=OK, 2=NI
C PSIA       SYSTEM PRESSURE, PSIA
C TF         TEMPERATURE, DEG F
C X1(I)      MOLE FRACTION OF I-TH COMPONENT IN LIQ PHASE 1
C X2(I)      MOLE FRACTION OF I-TH COMPONENT IN LIQ PHASE 2
C YDP(I)     MOLE FRACTION OF I-TH COMPONENT IN VAPOR
C ZDP(I)     MOLE FRACTION OF I-TH COMPONENT IN FEED
C
C REAL*8     ALPHA, BETA, PSIA, TF, X1(20), X2(20), YDP(20),
1 ZDP(20)
C REAL       DLG(20), GAM(1), G1(20), G2(20), Z(1)
C DIMENSION  KERR(1)
C
C DO 11 I     = 1, NC
C             DLG(I) = 0.0
11 ZDP(I) = Z(I)
C RETURN
C
C ENTRY      BUBBLE PRESSURE AT T
C IF (T.GT. TCM) GO TO 100
C PSIA = 14.696*PD
C IF (PSIA.LE. 0.0) PSIA = 30.0
C TF = 1.8*T - 459.67
C KERR(1) = MPBPP(ZDP, X2, X1, YDP, TF, PSIA, ALPHA, BETA, 2)
C PB = PSIA/14.696
C
C ENTRY      DEW PRESSURE AT T
C KERR(2) = MPBPP(ZDP, X2, X1, YDP, TF, PSIA, ALPHA, BETA, 3)
C PD = PSIA/14.696
C
C ENTRY      DEW GAS V, H, S AT T
C CALL SVGM (T, PD, VD)
C CALL SHGM (T, PD, VD, HD)
C CALL SSGM (T, PD, VD, SD)
C
C ENTRY      BUBBLE LIQUID V, H, S AT T
C CALL SVLM (T, PB, VB)
C IF (KGAM.EQ. 0) GO TO 55
C CALL SGAMVL (T + 1.0, Z)
C CALL MOVE (NC, GAM, G2)
C CALL SGAMVL (T - 1.0, Z)
C CALL MOVE (NC, GAM, G1)
C CALL SGAMVL (T, Z)
C DO 52 K     = 1, NC
52 DLG(K) = (G2(K) - G1(K))/(2.0*GAM(K))
55 CALL SHLB (T, PB, PD, DLG, HR)
CALL SSLB (T, PB, PD, GAM, DLG, SB)
100 RETURN
END

```

```

C      SUBROUTINE SFG1(A, B, R)
C      TITLE      GAS FUGACITY
C      REAL      A(1), B(1)
C      RETURN
C
C      GAS FUGACITY OF 1 AT T, P
C      ENTRY      SFGC(IC, T, P, FG)
C      = IC
C      CALL SVGC  (IC, T, P, V)
C      E          = P*V/(R*T) - 1.0 - ALOG(P*(V - B(1))/(R*T)) -
1              A(1)*ALOG(1.0 + B(1)/V)/(B(1)*R*T**1.5)
C      FG        = P*EXP(E)
C      RETURN
C      END

```

```

SUBROUTINE SGAMVL(GA, GAM, GK, /NC/)
      LIQUID ACTIVITY COEFFICIENTS
      SGAM 30

      INPUT      GA, GK, NC, TA, XV
      OUTPUT     GAM

      REAL       GA(20,20,3), GK(20,20,3), GAM(1), XV(1)
      REAL       A(20,20), C(20,20)

      RETURN
      ENTRY SGAMVL(TA, XV)
      NCM1 = NC - 1
      DO 31 I = 1, NCM1
        IP1 = I + 1
        DO 31 J = IP1, NC
          A(I,J) = GA(I,J,1) + GA(I,J,2)/TA + GA(I,J,3)*TA
          A(J,I) = GA(J,I,1) + GA(J,I,2)/TA + GA(J,I,3)*TA
          C(I,J) = GK(I,J,1) + GK(I,J,2)/TA + GK(I,J,3)*TA
          C(J,I) = C(I,J)
          SGAM 460
          SGAM 480
          SGAM 490
          SGAM 500
          SGAM 510
          SGAM 520
          SGAM 530
        XS = 0.0
        DO 41 I = 1, NC
          XS = XS + XV(I)
          SGAM 560
        DO 65 I = 1, NC
          XSMXI = XS - XV(I)
          IF (XSMXI) 51, 51, 60
          SGAM 590
          SGAM 600
          SGAM 610
          SGAM 620
          SGAM 630
          SGAM 640
          SGAM 650
          GO TO 65
        AI = 0.0
        BI = 0.0
        CI = 0.0
        DO 61 J = 1, NC
          IF (I .EQ. J) GO TO 61
          AI = AI + XV(J)*A(I,J)
          BI = BI + XV(J)*A(J,I)
          CI = CI + XV(J)*C(I,J)
          SGAM 670
        61 CONTINUE
        IF (AI .EQ. 0.0 .OR. BI .EQ. 0.0) GO TO 51
        AI = AI/XSMXI
        BI = BI/XSMXI
        CI = CI/XSMXI
        AX = ABS(AI)*XV(I)
        ZI = AX/(AX + ABS(BI)*XSMXI)
        GI = AI*(1.0 - ZI)**2
        ZI4 = 0.0
        IF (AI*BI .LT. 0.0) ZI4 = ZI*4.0
        GI = GI*(1.0 + CI*ZI*(ZI - 0.66666667) - ZI4)
        SGAM 710
        SGAM 720
        SGAM 730
        SGAM 740
        SGAM 750
        SGAM 770
        SGAM 780
        SGAM 790
        SGAM 800
        SGAM 810
        GAM(I) = EXP(GI)
        65 CONTINUE
      500 RETURN
      END

```



```

C      SUBROUTINE SHG1(NC, Y, CC, A, B, AM, BM, R, RM)
C      TITLE      = GAS ENTHALPY
C      REAL      A(1), B(1), C(5,20), CC(20,1), D(5), Y(1)
C
C      DO 12 I      = 1, NC
C          C(1,I) = 0.
C          C(2,I) = CC(I,1)
C          C(3,I) = CC(I,2)/2
C          C(4,I) = CC(I,3)/3
12      C(5,I) = CC(I,4)/4
C
C      DO 14 J      = 1, 5
C          D(J) = 0.0
14      DO 14 I      = 1, NC
C          D(J) = D(J) + Y(I)*C(J,I)
C      RETURN
C
C          GAS ENTHALPY OF I AT T, P
C      ENTRY      SHGC(IC, T, P, V, HG)
C          I      = IC
C          HG      = C(1,I) + T*(C(2,I) + T*(C(3,I) + T*(C(4,I) +
1      T*(C(5,I)))) + (P*V - R*T - 1.5*A(I)*
2      ALOG(1 + B(I)/V)/(SQRT(T)*B(I)))*RM/R
C      RETURN
C
C          GAS ENTHALPY OF MIXTURE AT T, P
C      ENTRY      SHGM(T, P, V, HG)
C          HG      = D(1) + T*(D(2) + T*(D(3) + T*(D(4) + T*(D(5)))) +
1      (P*V - R*T - 1.5*AM*ALOG(1 + BM/V)/(SQRT(T)*BM))
2      *RM/R
C      RETURN
C      END

```

```

C      SUBROUTINE      SHL1(NC, Y, R, RH, TC)
C      TITLE           = LIQUID ENTHALPY
C      REAL            DLG(1), TC(1), Y(1)
C      RETURN
C
C      BUBBLE LIQUID ENTHALPY AT T
ENTRY      SHLB(T, PB, PD, DLG, HLB)
      HLB      = 0.0
      DO 22 I      = 1, NC
      IF      (T .GT. TC(I)) GO TO 21
      CALL      SPSC      (I, T, PS)
      CALL      SVGC      (I, T, PS, VG)
      CALL      SHGC      (I, T, PS, VG, HG)
      CALL      SHVC      (I, T, HVAP)
      CALL      SVLC      (I, T, PB, VL)
      HLI      = HG - HVAP + VL*(PB - PS)*RH/R
      GO TO 22
21      CALL      SVGC      (I, T, PB, VG)
      CALL      SHGC      (I, T, PB, VG, HLI)
22      HLB      = HLB + Y(I)*(HLI - RH*T**2*DLG(I))
      RETURN
C
C      LIQUID ENTHALPY AT T, P
ENTRY      SHLL(T, P, PB, HLB, HL)
      CALL      SVLM      (T, PB, VL)
      CALL      SVLM      (T + 1.0, PB, VL2)
      CALL      SVLM      (T - 1.0, PB, VL1)
      HL      = HLB + (VL - T*(VL2 - VL1)/2)*(P - PB)*RH/R
      RETURN
END

```

```

C      SUBROUTINE SHV1(NC, HV1, T1, TC, TCM)
C      TITLE      = HEAT OF VAPORIZATION
C      REAL      HV1(1), TC(1), T1(1)
C      RETURN
C      HEAT OF VAPORIZATION OF I AT T
ENTRY  SHVC(I, T, HV)
      HV = 0.0
      IF (T .GE. TCM) RETURN
      HV = HV1(1)*((TCM - T)/(TCM - T1(1)))**0.38
RETURN
END

```

C	SUBROUTINE	SPS1(C)
C	TITLE	SATURATION PRESSURE
C	REAL	C(20,1)
C	RETURN	
C	ENTRY	VAPOR PRESSURE OF I AT T
	P	SPSC(I, T, P)
		= EXP(C(I,1) + C(I,2)/(T + C(I,3)))
	RETURN	
	END	

```

C      SUBROUTINE SSG1(NC, Y, CC, TR, PR, A, B, AM, BM, R, RH)
C      TITLE      = GAS ENTROPY
C
C      REAL      A(1), B(1), C(5,20), CC(20,1), D(5), Y(1)
C
C      DO 12 I      = 1, NC
C          C(2,I) = CC(I,2)
C          C(3,I) = CC(I,3)/2
C          C(4,I) = CC(I,4)/3
C          C(5,I) = CC(I,1)
C      12 C(1,I) = -TR*(C(2,I) + TR*(C(3,I) + TR*(C(4,I))))
C
C      DO 14 J      = 1, 5
C          D(J) = 0.
C      DO 14 I      = 1, NC
C      14 D(J) = D(J) + Y(I)*C(J,I)
C      RETURN
C
C          GAS ENTROPY OF I AT T, P
C      ENTRY SSGC(IC, T, P, V, SG)
C          I = IC
C          SG = C(1,I) + T*(C(2,I) + T*(C(3,I) + T*(C(4,I))) +
C              C(5,I)*ALOG(T/TR) - RH*ALOG(P/PR) +
C              RH*ALOG(P*(V - B(I))/(R*T)) -
C              0.5*A(I)*ALOG(1 + B(I)/V)/(T*1.5*B(I))*RH/R
C      RETURN
C
C          GAS ENTROPY OF MIXTURE AT T, P
C      ENTRY SSGM(T, P, V, SG)
C          SG = D(1) + T*(D(2) + T*(D(3) + T*(D(4))) +
C              D(5)*ALOG(T/TR) - RH*ALOG(P/PR) +
C              RH*ALOG(P*(V - BM)/(R*T)) -
C              0.5*AM*ALOG(1 + BM/V)/(T*1.5*BM))*RH/R
C      RETURN
C      END

```

```

C      SUBROUTINE  SSL1(NC, Y, R, RH, TC)
C      TITLE      = LIQUID ENTROPY
C
C      REAL        DLG(1), G(1), TC(1), Y(1)
C
C      RETURN
C
C      BUBBLE LIQUID ENTROPY AT T
C      ENTRY      SSLB(T, PB, PD, G, DLG, SLB)
C      CALL  SVGM  (T, PD, VG)
C      CALL  SSGM  (T, PD, VG, SG)
C      SLB      = SG
C      DO 22  I    = 1, NC
C      CALL  SHVC  (I, T, HV)
C      SLB      = SLB + Y(I)*(-HV/T + RH*(ALOG(G(I)*Y(I)) + T*DLG(I)))
22  CALL  SVLM  (T + 1.0, PB, VL2)
C      CALL  SVLM  (T - 1.0, PB, VL1)
C      SLB      = SLB - (VL2 - VL1) * (PB - PD) * RH / (2 * R)
C
C      RETURN
C
C      LIQUID ENTROPY AT T, P
C      ENTRY      SSLL(T, P, PB, SLR, SL)
C      CALL  SVLM  (T + 1.0, P, VL2)
C      CALL  SVLM  (T - 1.0, P, VL1)
C      SL      = SLR - (VL2 - VL1) * (P - PB) * RH / (2 * R)
C
C      RETURN
C      END

```



```

SUBROUTINE STB1(Z, NC, TCM, PCM, VCM, GAM, KERR, KGAM)
REAL*8 ALPHA, BETA, PSIA, TF, X1(20), X2(20), YDP(20),
1 ZDP(20)
REAL DLG(20), GAM(1), G1(20), G2(20), Z(1)
DIMENSION KERR(1)

C
DO 11 I = 1, NC
    DLG(I) = 0.0
11 ZDP(I) = Z(I)
RETURN

C
ENTRY STB(T, PB, VB, HB, SB)
IF (PB.GT. PCM) GO TO 100
PSIA = 14.696*PB
TF = 1.8*T - 459.67
KERR(1) = MPBPT(ZDP, X2, X1, YDP, TF, PSIA, ALPHA, BETA, 2)
T = (TF + 459.67)/1.8
DEW PRESSURE AT T
KERR(2) = MPBPP(ZDP, X2, X1, YDP, TF, PSIA, ALPHA, BETA, 3)
PD = PSIA/14.696
BUBBLE LIQUID V, H, S AT PB

C
CALL SVLM (T, PB, VB)
IF (KGAM.EQ. 0) GO TO 55
CALL SGAMVL (T + 1.0, Z)
CALL MOVE (NC, GAM, G2)
CALL SGAMVL (T - 1.0, Z)
CALL MOVE (NC, GAM, G1)
CALL SGAMVL (T, Z)
DO 52 K = 1, NC
52 DLG(K) = (G2(K) - G1(K))/(2.0*GAM(K))
55 CALL SHLB (T, PB, PD, DLG, HB)
CALL SSLB (T, PB, PD, GAM, DLG, SB)
100 RETURN
END

```

```

SUBROUTINE STD1(Z, NC, TCM, PCM, VCM, GAM, KERR, KGAM)
DIMENSION GAM(1), Z(1), KERR(1)
REAL*8 ALPHA, BETA, PSIA, TF, X1(20), X2(20), YDP(20),
1 ZDP(20)
C
DO 11 I = 1, NC
11 ZDP(I) = Z(I)
RETURN
C
ENTRY STD1(T, PD, VD, HD, SD)
IF (PD.GT. PCM) GO TO 100
PSIA = 14.696*PD
TF = 1.8*T - 459.67
KERR(2) = MP8PT(ZDP, X2, X1, YDP, TF, PSIA, ALPHA, BETA, 3)
T = (TF + 459.67)/1.8
C
CALL SVGM (T, PD, VD)
CALL SHGM (T, PD, VD, HD)
CALL SSGM (T, PD, VD, SD)
100 RETURN
END

```

```

C      SUBROUTINE  SVGI(NC, Y, TC, PC, R, A, B, AM, BM)
C      TITLE      = GAS VOLUME
C      REAL      A(1), B(1), PC(1), TC(1), Y(1)
C      CALL  ZRKC  (NC, TC, PC, H, A, B)
C      CALL  ZRKM  (NC, Y, A, B, AM, BM)
C      RETURN
C      GAS VOLUME OF I AT T, P
C      ENTRY      SVGC(I, T, P, V)
C      CALL  ZRKE  (T, P, A(I), B(I), Z, KERR)
C      V          = Z*R*T/P
C      RETURN
C      GAS VOLUME OF MIXTURE AT T, P
C      ENTRY      SVGM(T, P, V)
C      CALL  ZRKE  (T, P, AM, BM, Z, KERR)
C      V          = Z*R*T/P
C      RETURN
C      END

```

```

C      SUBROUTINE SVL1(NC, Y, DL1, T1, TC, PC, R, TCM, PCM)
C      TITLE      = LIQUID VOLUME
C
C      REAL      C(2,20), DC(20), DL1(1), PC(1), TC(1), T1(1), Y(1)
C
C          DCM      = 3*PCM/(R*TCM)
C      DO 12 I      = 1, NC
C          CALL SPSC (I, T1(I), P)
C          CALL SVGC (I, T1(I), P, VG)
C          C(2,I) = (2*DCM - DL1(I) - 1/VG)/(TCM - T1(I))
12      C(1,I) = 2*DCM - C(2,I)*TCM
C      RETURN
C
C          LIQUID VOLUME OF I AT T
C      ENTRY      SVLC(IC, T, P, V)
C          I      = IC
C          IF (T .GE. TCM) GO TO 21
C          CALL SPSC (I, T, PS)
C          CALL SVGC (I, T, PS, VG)
C          V      = 1/(C(1,I) + C(2,I)*T - 1/VG)
C      RETURN
21      V      = 1/DCM
C      RETURN
C
C          LIQUID VOLUME OF MIXTURE AT T
C      ENTRY      SVLM(T, P, VM)
C          IF (T .GE. TCM) GO TO 34
C          VM      = 0.0
C          DO 32 I      = 1, NC
C          CALL SPSC (I, T, PS)
C          CALL SVGC (I, T, PS, VG)
C          VL      = 1/(C(1,I) + C(2,I)*T - 1/VG)
32      VM      = VM + Y(I)*VL
C      RETURN
34      VM      = 1/DCM
C      RETURN
C      END

```

8. DESCRIPTION OF LIBRARY SUBPROGRAMS

8.1 DATE4

This assembly language subroutine provides the current date. The calling sequence is

```
CALL DATE4(DATE)
```

On return, the eight characters addressed by DATE will contain mm/dd/yy in character form.

8.2 HEADER

This utility subroutine controls the output page count, initializes the line count, and prints a two line heading on each output page. The calling sequence is

```
CALL HEADER(KS)
```

If KS is less than zero, the routine set the numeric part of the program E number from -KS. If K equals 1, the internal page counter is incremented, the page heading is written on a new page, and the line count is set to 2.

8.3 KTBL

This utility subprogram controls the printing to tables. The calling sequence is

```
CALL KTBL(LM,LS,NB)
```

where LM = number of lines in the table title
LS = number of lines in the table subtitle. If the table is continued onto a new page, the calling routine reprints the subtitle
NB = number of lines per group. Groups are separated by a blank line.

The function entry point KTBL1 (Dummy) increments the line counter, inserts blank lines between groups, and continues the table on a new page with a page heading printed by subroutine HEADER. The function value of 1 is a request for calling routine to reprint the table subtitle.

8.4 MASS

This subroutine converts mole amounts to mass amounts and computes the mixture molecular weight. The calling sequence is

CALL MASS(NC,WMC,Y,YS,X,XS,WMM)

where NC = number of components
WMC = array of component molecular weights
WMM = mixture molecular weight
X = array of component masses
XS = total mass of mixture
Y = array of component moles
YS = total moles of mixture

8.5 MOVE

This utility subroutine transfers N elements of array X to array Y. The calling sequence is

CALL MOVE(N,X,Y)

8.6 MPBPP

This function either computes the bubble point pressure at a specified temperature and liquid composition or it computes the dew point pressure at a specified temperature and gas composition. The invocation is

MPBPP(Z,S,X,Y,T,P,A,B,K)

where A = superfluous argument
B = superfluous argument
K = calculation code: 2 = bubble point pressure
3 = dew point pressure
P = bubble point pressure or dew point pressure, psi
S = scratch array of NC elements
T = specified temperature, °F
X = computed array of liquid mole fractions
Y = computed array of gas mole fractions
Z = specified array of liquid or gas mole fractions

The function name MPBPP is used as an error indicator: 1 = success, 2 = failure.

8.7 MPBPT

This function either computes the bubble point temperature at a specified pressure and liquid composition or it computes the dew point temperature at a specified pressure and gas composition. The invocation is

MPBPT(Z,S,X,Y,T,P,A,B,K)

where A = superfluous argument
 B = superfluous argument
 K = calculation code: 2 = bubble point temperature,
 3 = dew point temperature
 P = specified pressure, psi
 S = scratch array of NC elements
 T = computed bubble point temperature or dew point
 temperature, °F
 X = computed array of liquid mole fractions
 Y = computed array of gas mole fractions
 Z = specified array of liquid or gas mole fractions

The function name MPBPT is used as an error indicator: 1 = success,
 2 = failure.

8.8 NORM

This subroutine normalizes the elements of an array X. The
 calling sequence is

CALL NORM(N,X,S,Y)

where N = number of elements
 S = computed sum of the elements of X
 X = given array
 Y = normalized array with elements X_i/S .

8.9 UCP

This subprogram converts pressure units. The calling sequence is

CALL UCP(N,KI,KØ,PI,PØ)

where KI = pressure unit for PI: 1 = atm, 2 = psi, 3 = mmHg
 KØ = pressure unit for PØ: 1 = atm, 2 = psi, 3 = mmHg
 N = number of elements in PI and PØ
 PI = array of specified pressures
 PØ = array of computed pressures

8.10 UCT

This subprogram converts temperature units. The calling sequence is

CALL UCT(N,KI,KØ,TI,TØ)

where KI = temperature unit for TI: 1 = C, 2 = F, 3 = K, 4 = R
 KØ = temperature unit for TØ: 1 = C, 2 = F, 3 = K, 4 = R
 N = number of elements in TI and TØ
 TI = array of specified temperatures
 TØ = array of computed temperatures

8.11 ZERO

This utility subroutine zeros all of the elements of an array X with indexes from I1 to I2 inclusive. The calling sequence is

CALL ZERO(X,I1,I2)

8.12 ZRKE

This subroutine computes the compressibility factor at a specified temperature and pressure using specified values for the Redlich-Kwong equation of state parameters. The calling sequence is

CALL ZRKE(T,P,A,B,Z,K)

where A = Redlich-Kwong equation parameter, $\text{atm-K}^{0.5}\text{-cm}^6/\text{gmol}^2$
B = Redlich-Kwong equation parameter, cm^3/gmol
K = return code: 0 = Z computed at T and P, 1 = Z computed
T and the saturation pressure at T because of the
absence of a vapor root at very low reduced pressures
P = specified pressure, atm
T = specified temperature, °K
Z = computed compressibility factor.

8.13 ZRKC

This subroutine computes Redlich-Kwong equation parameters for pure components. Inputs are the critical temperature and the critical pressure of the components. The calling sequence is

CALL ZRKC(NC,TC,PC,R,A,B)

where A = array of component Redlich-Kwong parameters,
 $\text{atm-K}^{0.5}\text{-cm}^6/\text{gmol}^2$
B = array of component Redlich-Kwong parameters, cm^3/gmol
NC = number of components
PC = array of component critical pressures, atm
R = gas constant, $82.0575 \text{ atm cm}^3/\text{gmol-K}$
TC = array of component critical temperatures, °K.

8.14 ZRKM

This subroutine computes the Redlich-Kwong parameters for a mixture by combining the pure component parameters. The calling sequence is

CALL ZRKM(NC,Y,A,B,AM,BM)

where A = array of component Redlich-Kwong parameters,
 $\text{atm-K}^{0.5}\text{-cm}^6/\text{gmol}^2$
AM = mixture Redlich-Kwong parameter, $\text{atm-K}^{0.5}\text{-cm}^6/\text{gmol}^2$
B = array of component Redlich-Kwong parameters, cm^3/gmol
BM = mixture Redlich-Kwong parameter, cm^3/gmol
NC = number of components
Y = array of component mole fractions.

9. FILLED-IN INPUT DATA LISTS

Monsanto	INPUT DATA SHEET 1 OF 3 THERMODYNAMIC PROPERTIES OF MULTICOMPONENT FLUIDS	BY _____ DATE _____
Program E1393		

LIST 1: PROBLEM-SET IDENTIFICATION and LIST 2: CASE IDENTIFICATION (Optional)
1 <u>1000 KINETIC CYCLE TEST PROBLEM</u> 2 <u>00</u>

LIST 3: Temperature Grid	
Description	Entry
List Number	3
Temperature Unit: 0=C, 1=F, 2=K, 3=R	1
Temperature Grid Lower Limit	200
Temperature Grid Upper Limit	800
Temperature Grid Increment	25
Spare Code	0

LIST 4: Pressure Grid	
Description	Entry
List Number	4
Pressure Unit: 0=atm, 1=psi, 2=mmHg	0
Number of Pressures (50 max)	8
Pressures	
1-5	1
6-10	50
11-15	80
16-20	100
21-25	10
26-30	20
31-35	
36-40	
41-45	
46-50	

LIST 5: SYSTEM COMPOSITION	
Description	Entry
List Number	5
Input Composition Code (1 = Mass Units, 2 = Mole Units)	2
Number of Components (20 Max)	2
Comp. No.	Composition Data in Fractions, Percents, or Flows
1-5	60
6-10	40
11-15	
16-20	

‡ Start New Card

Monsanto

INPUT DATA SHEET 2 OF 3
THERMODYNAMIC PROPERTIES
OF MULTICOMPONENT FLUIDS

Program E1393

BY _____ DATE _____

LIST 6: MOLECULAR WEIGHTS AND ANTOINE CONSTANTS

Description						Entry
List Number						± 6
Number of Components (20 Max)						± 2
Component		Molecular Weight	Antoine Constants *			
Number	Name		a	b	c	
1	± ETHANOL	46.07	11.4255	-3309.61	-41.8291	
2	± WATER	18.016	12.0352	-4030.17	-38.15	
3	±					
4	±					
5	±					

* $\ln P^\circ = a + b/(T + c)$ with vapor pressure (P°) in atm and temperature (T) in °K.LIST 7: LIQUID ACTIVITY COEFFICIENT DATA: A_{ij} (Optional)

Description									Entry
List Number									± 7
Number of Binary Pairs Entered Below *									± 1
Equation Type, 1 = Van Laar †									1
Pair Number	Component Numbers		Temperature Coefficients for A_{ij}			Temperature Coefficients for A_{ji}			
	i	j	a_{ij}	b_{ij}	c_{ij}	a_{ji}	b_{ji}	c_{ji}	
1	1	2	9.8264	-1573.1	-0.02482	-1.3566	552.74	-0.0168433	
2									
3									
4									
5									

* Maximum number of binary pairs = $N(N-1)/2$ where N is the number of components. Entries for ideal pairs may be omitted.† $A_{ij} = a_{ij} + b_{ij}/T + c_{ij}T$ where T is in °K and $A_{ij} = \ln \gamma_i^\infty$.LIST 8: LIQUID ACTIVITY COEFFICIENT DATA; THIRD PARAMETER C_{ij} (Optional)

Description						Entry
List Number						± 8
Number of Binary Pairs with Third Parameter Entries						±
Equation Type, 1 = Van Laar *						
Pair Number	Component Numbers		Temperature Coefficients for C_{ij}			
	i	j	a_{ij}	b_{ij}	c_{ij}	
1						
2						
3						
4						
5						

* $C_{ij} = a_{ij} + b_{ij}/T + c_{ij}T$ where T is in °K. $C_{ji} = C_{ij}$.

‡ Start New Card

Monsanto

 INPUT DATA SHEET 3 OF 3
 THERMODYNAMIC PROPERTIES
 OF MULTICOMPONENT FLUIDS

Program E1993

BY _____ DATE _____

LIST 9: Ideal Gas Heat Capacity Constants

Description					Entry
List Number					9
Number of Components (20 Max)					2
Component Number	Ideal Gas Heat Capacity Constants*				
	a	b	c	d	
1	3.578	49.847E-3	-169.91E-7	0	
2	7.136	2.64E-3	.0459E-6	0	
3					
4					
5					

* $C_p = a + bT + cT^2 + dT^3$ C_p in cal/gmol-°K, T in °K.

LIST 10: Critical Properties, Heat of Vaporization, Liquid Density

Description							Entry
List Number							10
Number of Components (20 Max)							2
Component Number	Critical Temp °K	Critical Pressure atm	Heat of Vaporization at T_c cal/gmol	T_c for ΔH_v °K	Liquid Density at T_c gm/cm ³	T_c for ρ_L °K	
1	516.2	68	9260	351.44	.78504	298.15	
2	647.3	218.3	9716.7	373.15	.9584	298.15	
3							
4							
5							

LIST 99: END OF CASE CONTROL

99

Start New Card

10. OUTPUT FROM DATA LISTED IN SECTION 9

RANKINE CYCLE TEST PROBLEM 1.1

E1393 P 1
11/30/72

COMPOSITION	MOLE %	MASS %	MOLE WT
1 ETHANOL	60.000	79.321	46.07
2 WATER	40.000	20.679	18.02
MIXTURE	100.000	100.000	34.85

THERMODYNAMIC PROPERTIES AT SATURATION

TEMP T	P	D	H	S
DEG F	PSI	LB/FT3	BTU/LB	BTU/LB-F
200.00	24.27	47.34	161.0	0.2526
225.00	39.02	45.99	186.6	0.2897
250.00	60.35	44.57	212.9	0.3265
275.00	90.25	43.07	239.9	0.3629
300.00	131.02	41.47	267.7	0.3992
325.00	185.28	39.74	296.6	0.4354
350.00	256.04	37.86	326.6	0.4717
375.00	346.74	35.77	358.1	0.5085
400.00	461.53	33.42	391.5	0.5443
425.00	605.87	30.68	427.5	0.5856
450.00	789.29	27.25	466.9	0.6278
475.00	1050.74	21.09	611.8	0.6722
500.00	1833.90	16.80	647.9	0.4571

TEMP T	P	D	H	S
DEG F	PSI	LB/FT3	BTU/LB	BTU/LB-F
200.00	22.87	0.1146	635.2	1.019
225.00	37.05	0.1804	645.1	1.007
250.00	57.71	0.2741	654.9	0.9961
275.00	86.83	0.4044	664.4	0.9870
300.00	126.74	0.5818	673.6	0.9790
325.00	180.12	0.8200	682.2	0.9718
350.00	250.01	1.137	690.2	0.9650
375.00	339.95	1.589	697.2	0.9584
400.00	454.10	2.125	703.0	0.9515
425.00	597.92	2.905	706.7	0.9435
450.00	780.45	4.054	707.1	0.9329
475.00	1033.90	6.319	696.9	0.9118
500.00	1521.40	13.81	648.9	0.8521

RANKINE CYCLE TEST PROBLEM 1.1

E1393 P 2
11/30/72

THERMODYNAMIC PROPERTIES AT SATURATION

TEMP	BUBBLE POINT LIQUID - - - - -			
T	P	D	H	S
DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
175.78	14.70	48.60	136.7	0.2163
209.82	29.39	46.82	171.0	0.2672
261.98	73.48	43.86	225.7	0.3440
304.09	146.96	40.92	276.9	0.4109
361.18	293.92	36.95	340.5	0.4841
443.23	734.80	28.28	455.9	0.6160
483.73	1175.68	19.70	620.7	0.6833

TEMP	DEW POINT GAS - - - - -			
T	P	D	H	S
DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
178.90	14.70	0.7566E-01	626.8	1.031
212.73	29.39	0.1451	640.3	1.012
264.54	73.48	0.3449	660.5	0.9907
310.31	146.96	0.6718	677.2	0.9760
362.47	293.92	1.341	694.0	0.9616
444.32	734.80	3.745	707.4	0.9357
485.23	1175.68	9.053	676.4	0.8862

RANKINE CYCLE TEST PROBLEM 1.1

E1393 P 3
11/30/72

COMPOSITION	MOLE %	MASS %	MOLE WT
1 STEAM	40.000	79.321	46.07
2 WATER	40.000	20.679	18.02
MIXTURE	100.000	100.000	34.85

THERMODYNAMIC PROPERTIES IN SINGLE PHASE REGION

TEMP	P	D	H	S
T DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
200.00	14.70	0.7316E-01	635.8	1.045
225.00	14.70	0.7041E-01	646.8	1.061
250.00	14.70	0.6787E-01	657.9	1.077
275.00	14.70	0.6550E-01	669.3	1.093
300.00	14.70	0.6330E-01	680.9	1.108
325.00	14.70	0.6124E-01	692.7	1.123
350.00	14.70	0.5932E-01	704.8	1.139
375.00	14.70	0.5751E-01	717.0	1.153
400.00	14.70	0.5581E-01	729.5	1.168
425.00	14.70	0.5421E-01	742.1	1.183
450.00	14.70	0.5270E-01	755.0	1.197
475.00	14.70	0.5127E-01	768.1	1.211
500.00	14.70	0.4992E-01	781.4	1.225
525.00	14.70	0.4864E-01	794.9	1.239
550.00	14.70	0.4743E-01	808.5	1.253
575.00	14.70	0.4627E-01	822.4	1.266
600.00	14.70	0.4517E-01	836.5	1.280
625.00	14.70	0.4412E-01	850.7	1.293
650.00	14.70	0.4312E-01	865.2	1.306
675.00	14.70	0.4216E-01	879.8	1.319
700.00	14.70	0.4124E-01	894.6	1.332
725.00	14.70	0.4037E-01	909.5	1.345
750.00	14.70	0.3953E-01	924.7	1.358
775.00	14.70	0.3872E-01	940.0	1.370
800.00	14.70	0.3795E-01	955.5	1.383
200.00	29.39	47.34	161.0	0.2526
225.00	29.39	0.1423	645.7	1.020
250.00	29.39	0.1370	656.9	1.036
275.00	29.39	0.1321	668.3	1.052
300.00	29.39	0.1276	680.0	1.068
325.00	29.39	0.1234	691.9	1.083
350.00	29.39	0.1194	703.9	1.098
375.00	29.39	0.1157	716.2	1.113
400.00	29.39	0.1122	728.7	1.128
425.00	29.39	0.1090	741.4	1.143

RANKINE CYCLE TEST PROBLEM 1.1

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11/30/72

TEMP T DEG F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-F
450.00	29.39	0.1059	754.3	1.157
475.00	29.39	0.1030	767.5	1.171
500.00	29.39	0.1002	780.8	1.185
525.00	29.39	0.9764E-01	794.3	1.199
550.00	29.39	0.9517E-01	808.0	1.213
575.00	29.39	0.9283E-01	821.9	1.227
600.00	29.39	0.9060E-01	835.9	1.240
625.00	29.39	0.8848E-01	850.2	1.253
650.00	29.39	0.8645E-01	864.7	1.266
675.00	29.39	0.8452E-01	879.3	1.280
700.00	29.39	0.8267E-01	894.1	1.292
725.00	29.39	0.8090E-01	909.1	1.305
750.00	29.39	0.7921E-01	924.3	1.318
775.00	29.39	0.7759E-01	939.6	1.330
800.00	29.39	0.7603E-01	955.1	1.343
200.00	73.48	47.34	161.0	0.2524
225.00	73.48	45.99	186.6	0.2895
250.00	73.48	44.57	212.9	0.3264
275.00	73.48	0.3393	665.3	0.9974
300.00	73.48	0.3268	677.2	1.013
325.00	73.48	0.3153	689.2	1.029
350.00	73.48	0.3046	701.4	1.044
375.00	73.48	0.2946	713.8	1.059
400.00	73.48	0.2853	726.4	1.074
425.00	73.48	0.2767	739.3	1.089
450.00	73.48	0.2685	752.3	1.103
475.00	73.48	0.2609	765.5	1.118
500.00	73.48	0.2537	778.9	1.132
525.00	73.48	0.2469	792.5	1.146
550.00	73.48	0.2404	806.2	1.160
575.00	73.48	0.2343	820.2	1.173
600.00	73.48	0.2285	834.4	1.187
625.00	73.48	0.2231	848.7	1.200
650.00	73.48	0.2178	863.2	1.213
675.00	73.48	0.2128	877.9	1.226
700.00	73.48	0.2081	892.8	1.239
725.00	73.48	0.2036	907.8	1.252
750.00	73.48	0.1992	923.0	1.265
775.00	73.48	0.1951	938.4	1.278
800.00	73.48	0.1911	953.9	1.290

RANKINE CYCLE TEST PROBLEM 1.1

E1393 P 5
11/30/72

TEMP T DEG F	P PSI	U LB/FT3	H BTU/LB	S BTU/LB-F
200.00	146.96	47.34	161.1	0.2521
225.00	146.96	45.99	186.7	0.2892
250.00	146.96	44.57	212.9	0.3260
275.00	146.96	43.07	239.9	0.3624
300.00	146.96	41.47	267.7	0.3991
325.00	146.96	0.6562	684.5	0.9853
350.00	146.96	0.6315	697.0	1.001
375.00	146.96	0.6088	709.6	1.016
400.00	146.96	0.5879	722.5	1.032
425.00	146.96	0.5685	735.5	1.046
450.00	146.96	0.5505	748.7	1.061
475.00	146.96	0.5337	762.1	1.076
500.00	146.96	0.5181	775.6	1.090
525.00	146.96	0.5033	789.4	1.104
550.00	146.96	0.4895	803.3	1.119
575.00	146.96	0.4765	817.4	1.132
600.00	146.96	0.4641	831.6	1.146
625.00	146.96	0.4525	846.1	1.159
650.00	146.96	0.4415	860.7	1.172
675.00	146.96	0.4310	875.5	1.185
700.00	146.96	0.4210	890.4	1.199
725.00	146.96	0.4115	905.6	1.211
750.00	146.96	0.4024	920.9	1.224
775.00	146.96	0.3938	936.3	1.237
800.00	146.96	0.3855	951.9	1.249
200.00	293.92	47.34	161.3	0.2514
225.00	293.92	45.99	186.8	0.2885
250.00	293.92	44.57	212.9	0.3252
275.00	293.92	43.07	239.8	0.3617
300.00	293.92	41.47	267.6	0.3980
325.00	293.92	39.74	296.4	0.4345
350.00	293.92	37.86	326.5	0.4713
375.00	293.92	1.312	700.4	0.9694
400.00	293.92	1.257	713.9	0.9852
425.00	293.92	1.208	727.4	1.001
450.00	293.92	1.163	741.1	1.016
475.00	293.92	1.122	754.9	1.031
500.00	293.92	1.084	768.8	1.046
525.00	293.92	1.049	782.9	1.060
550.00	293.92	1.017	797.1	1.074

RANKINE CYCLE TEST PROBLEM 1.1

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11/30/72

TEMP T	P	D	H	S
DEG F	PSI	LB/FT ³	BTU/LB	BTU/LB-F
575.00	293.92	0.9868	811.5	1.089
600.00	293.92	0.9586	826.0	1.102
625.00	293.92	0.9323	840.7	1.116
650.00	293.92	0.9075	855.6	1.130
675.00	293.92	0.8842	870.6	1.143
700.00	293.92	0.8622	885.7	1.156
725.00	293.92	0.8414	901.0	1.169
750.00	293.92	0.8216	916.5	1.182
775.00	293.92	0.8028	932.1	1.195
800.00	293.92	0.7850	947.9	1.208
200.00	734.80	47.34	161.7	0.2495
225.00	734.80	45.99	187.1	0.2863
250.00	734.80	44.57	213.1	0.3228
275.00	734.80	43.07	239.7	0.3589
300.00	734.80	41.47	267.2	0.3949
325.00	734.80	39.74	295.5	0.4307
350.00	734.80	37.86	325.0	0.4664
375.00	734.80	35.77	355.9	0.5036
400.00	734.80	33.42	389.1	0.5417
425.00	734.80	30.68	425.6	0.5826
450.00	734.80	3.679	711.3	0.9400
475.00	734.80	3.431	727.9	0.9580
500.00	734.80	3.231	744.0	0.9751
525.00	734.80	3.063	760.0	0.9915
550.00	734.80	2.918	775.8	1.007
575.00	734.80	2.792	791.5	1.023
600.00	734.80	2.680	807.2	1.038
625.00	734.80	2.579	823.0	1.052
650.00	734.80	2.488	838.8	1.067
675.00	734.80	2.405	854.6	1.081
700.00	734.80	2.329	870.6	1.095
725.00	734.80	2.259	886.6	1.109
750.00	734.80	2.193	902.7	1.122
775.00	734.80	2.133	918.9	1.135
800.00	734.80	2.076	935.2	1.148
200.00	1175.68	47.34	162.2	0.2476
225.00	1175.68	45.99	187.4	0.2842
250.00	1175.68	44.57	213.2	0.3204
275.00	1175.68	43.07	239.6	0.3562
300.00	1175.68	41.47	266.7	0.3917

HANKING CYCLE TEST PROBLEM 1.1

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11/30/72

TEMP T	D	D	M	S
DEG F	PSI	LB/FT3	BTU/LB	BTU/LB-F
325.00	1175.68	39.74	294.6	0.4270
350.00	1175.68	37.86	323.5	0.4623
375.00	1175.68	35.77	353.5	0.4979
400.00	1175.68	33.42	385.2	0.5343
425.00	1175.68	30.68	419.0	0.5721
450.00	1175.68	27.25	455.4	0.6123
475.00	1175.68	21.09	605.9	0.6647
500.00	1175.68	7.414	700.7	0.9117
525.00	1175.68	6.358	725.7	0.9375
550.00	1175.68	5.742	746.6	0.9584
575.00	1175.68	5.303	765.7	0.9772
600.00	1175.68	4.962	784.0	0.9946
625.00	1175.68	4.684	801.8	1.011
650.00	1175.68	4.449	819.2	1.027
675.00	1175.68	4.247	836.4	1.042
700.00	1175.68	4.070	853.6	1.057
725.00	1175.68	3.912	870.6	1.072
750.00	1175.68	3.771	887.7	1.086
775.00	1175.68	3.643	904.7	1.100
800.00	1175.68	3.526	921.7	1.114
200.00	1469.60	47.34	162.5	0.2463
225.00	1469.60	45.99	187.6	0.2828
250.00	1469.60	44.57	213.3	0.3184
275.00	1469.60	43.07	239.5	0.3544
300.00	1469.60	41.47	266.4	0.3896
325.00	1469.60	39.74	294.1	0.4245
350.00	1469.60	37.86	322.5	0.4593
375.00	1469.60	35.77	351.9	0.4942
400.00	1469.60	33.42	382.6	0.5294
425.00	1469.60	30.68	414.6	0.5652
450.00	1469.60	27.25	446.6	0.6005
475.00	1469.60	21.09	591.9	0.6470
500.00	1469.60	13.30	652.2	0.8562
525.00	1469.60	13.46	664.2	0.8686
550.00	1469.60	9.172	714.7	0.9193
575.00	1469.60	7.846	741.8	0.9459
600.00	1469.60	7.060	764.2	0.9673
625.00	1469.60	6.503	784.7	0.9863
650.00	1469.60	6.072	804.0	1.004
675.00	1469.60	5.724	822.7	1.021

RANKINE CYCLE TEST PROBLEM 1.1

E1393 P. A
11/30/72

TEMP T DEG F	P PSI	D LB/FT ³	H BTU/LB	S BTU/LB-F
700.00	1469.60	5.431	841.0	1.037
725.00	1469.60	5.180	859.0	1.052
750.00	1469.60	4.961	876.9	1.067
775.00	1469.60	4.766	894.6	1.081
800.00	1469.60	4.592	912.3	1.096

11. BLANK INPUT DATA SHEETS FOR PROGRAM E1393

Monsanto	INPUT DATA SHEET 1 OF 3	
	THERMODYNAMIC PROPERTIES OF MULTICOMPONENT FLUIDS	BY _____ DATE _____
Program	E1393	

LIST 1: PROBLEM-SET IDENTIFICATION	and	LIST 2: CASE IDENTIFICATION (Optional)
1 bb _____ 2 bb _____		

LIST 3: Temperature Grid		Entry
Description		
List Number		3
Temperature Unit: 0=C, 1=F, 2=K, 3=R		
Temperature Grid Lower Limit		
Temperature Grid Upper Limit		
Temperature Grid Increment		
Spare Code		

LIST 4: Pressure Grid		Entry
Description		
List Number		4
Pressure Unit: 0=atm, 1=psi, 2=mmHg		
Number of Pressures (50 max)		
Pressures		
1-5		
6-10		
11-15		
16-20		
21-25		
26-30		
31-35		
36-40		
41-45		
46-50		

LIST 5: SYSTEM COMPOSITION		Entry
Description		
List Number		5
Input Composition Code (1 = Mass Units, 2 = Mole Units)		
Number of Components (20 Max)		
Comp. No.	Composition Data in Fractions, Percents, or Flows	
1-5		
6-10		
11-15		
16-20		

† Start New Card

Monsanto

INPUT DATA SHEET 2 OF 3 THERMODYNAMIC PROPERTIES OF MULTICOMPONENT FLUIDS

Program E:293

BY _____ DATE _____

LIST 6: MOLECULAR WEIGHTS AND ANTOINE CONSTANTS

Description						Entry
List Number						± 6
Number of Components (20 Max)						±
Component		Molecular Weight	Antoine Constants *			
Number	Name		a	b	c	
1	± _____	_____	_____	_____	_____	
2	± _____	_____	_____	_____	_____	
3	± _____	_____	_____	_____	_____	
4	± _____	_____	_____	_____	_____	
5	± _____	_____	_____	_____	_____	

* $\ln P^s = a + b/(T + c)$ with vapor pressure (P^s) in atm and temperature (T) in °K.LIST 7: LIQUID ACTIVITY COEFFICIENT DATA: A_{ij} (Optional)

Description									Entry
List Number									± 7
Number of Binary Pairs Entered Below *									±
Equation Type, 1 = Van Laar †									±
Pair Number	Component Numbers		Temperature Coefficients for A_{ij}			Temperature Coefficients for A_{ji}			
	i	j	a_{ij}	b_{ij}	c_{ij}	a_{ji}	b_{ji}	c_{ji}	
1	_____	_____	_____	_____	_____	_____	_____	_____	
2	_____	_____	_____	_____	_____	_____	_____	_____	
3	_____	_____	_____	_____	_____	_____	_____	_____	
4	_____	_____	_____	_____	_____	_____	_____	_____	
5	_____	_____	_____	_____	_____	_____	_____	_____	

* Maximum number of binary pairs = $N(N-1)/2$ where N is the number of components. Entries for ideal pairs may be omitted.† $A_{ij} = a_{ij} + b_{ij}/T + c_{ij}T$ where T is in °K and $A_{ij} = \ln \gamma_i^\infty$.LIST 8: LIQUID ACTIVITY COEFFICIENT DATA; THIRD PARAMETER C_{ij} (Optional)

Description						Entry
List Number						± 8
Number of Binary Pairs with Third Parameter Entries						±
Equation Type, 1 = Van Laar *						±
Pair Number	Component Numbers		Temperature Coefficients for C_{ij}			
	i	j	a_{ij}	b_{ij}	c_{ij}	
1	_____	_____	_____	_____	_____	
2	_____	_____	_____	_____	_____	
3	_____	_____	_____	_____	_____	
4	_____	_____	_____	_____	_____	
5	_____	_____	_____	_____	_____	

* $C_{ij} = a_{ij} + b_{ij}/T + c_{ij}T$ where T is in °K. $C_{ji} = C_{ij}$.

† Start New Card

Monsanto

INPUT DATA SHEET 3 OF 3
THERMODYNAMIC PROPERTIES
OF MULTICOMPONENT FLUIDS

Program E1393

BY _____ DATE _____

LIST 9: Ideal Gas Heat Capacity Constants

Description					Entry
List Number					† 9
Number of Components (20 Max)					‡
Component Number	Ideal Gas Heat Capacity Constants*				
	a	b	c	d	
1					
2					
3					
4					
5					

* $C_p = a + bT + cT^2 + dT^3$ C_p in cal/gmol-°K. T in °K.

LIST 10: Critical Properties, Heat of Vaporization, Liquid Density

Description							Entry
List Number							† 10
Number of Components (20 Max)							‡
Component Number	Critical Temp °K	Critical Pressure atm	Heat of Vaporization at T_c cal/gmol	T_c for ΔH_v °K	Liquid Density at T_c gm/cm ³	T_c for ρ_L °K	
1							
2							
3							
4							
5							

LIST 99: END OF CASE CONTROL

† 99

* Start New Card

APPENDIX L

COMPUTER PROGRAM E-1375

*Isoteniscope Data Analysis: The determination
van Laar parameters for binary liquid mixtures
by vapor pressure vs. temperature measurements.*

1. SCOPE

This program is designed to estimate parameters of the van Laar equation for liquid phase activity coefficients from a minimum of experimental data. Vapor pressure data, in the form of Antoine equation constants, for the two pure components and two or more binary mixture compositions are the primary input data. The output consists of the van Laar constants giving the best fit to the vapor pressures of the mixtures at a number of predetermined temperature levels.

The program is limited to binary systems for which the van Laar equation gives an adequate representation of the activity coefficient.

2. MODEL

2.1 Definitions

A,B,C,	Constants in the Antoine equation for vapor pressure
A ₁₂ ,A ₂₁ ,E _a	Parameters in the van Laar equation for liquid phase activity coefficients
a,b	Constants in the Redlich-Kwong equation of state for gas phase
M	Molecular weight
P	Total vapor pressure over a liquid mixture, atm.
p ^o	Vapor pressure of a pure component liquid, atm.
P _c	Critical pressure, atm.
R	Gas constant, 82.0557 cm ³ atm/gmol ^o K
T	Temperature, ^o K
T _c	Critical temperature, ^o K
v	Volume of gas mixture, cm ³ /gmol
v _L	Volume of pure component liquid, cm ³ /gmol
x	Mole fraction in liquid mixture
y	Mole fraction in vapor mixture

z	Modified mole fraction in van Laar equation
α, β, ξ	Constants in liquid density polynomial
γ	Liquid phase activity coefficient
ρ	Liquid density, g/cm ³
ϕ^0	Fugacity coefficient for pure component at its vapor pressure
$\hat{\phi}$	Fugacity ratio of given component in the vapor mixture at pressure, P.
Subscripts	
1,2,1	Component number designations
m	Mixture property designation

2.2 Computation Method

The program performs a least squares regression analysis, varying A_{12} and A_{21} of the van Laar equations, until the best fit is obtained when experimental and calculated total vapor pressures of the mixtures are compared. Details of the calculations are as follows:

2.2.1 Experimental and Pure Component Vapor Pressures

Experimental total vapor pressures are computed by the Antoine Eq.:

$$\ln P = A_m + B_m/(T+C_m) \quad (1)$$

Pure component vapor pressures are also computed by Antoine Eq.:

$$\ln p_i^0 = A_i + B_i/(T+C_i) \quad (2)$$

The values of A_m, B_m, C_m for each mixture composition, and A_i, B_i, C_i for each component are input data to the program.

2.2.2 Calculated Mixture Vapor Pressure

The partial pressure of each component is calculated by

$$p_{y1} = \gamma_1 x_1 \phi_1^0 p_1^0 \exp (v_{L1}[P-p_1^0]/RT/\hat{\phi}_1) \quad (3)$$

The total pressure is the sum of the partial pressures

$$P = \gamma_1 x_1 \phi_1^0 p_1^0 \exp (v_{L1}[P-p_1^0]/RT)/\hat{\phi}_1 + \gamma_2 x_2 \phi_2^0 p_2^0 \exp (v_{L2}[P-p_2^0]/RT)/\hat{\phi}_2 \quad (4)$$

2.2.3 Liquid Volumes

Liquid volumes are calculated from a liquid density polynomial

$$\rho_1 = \alpha_1 + \beta_1 T + \xi_1 T^2 \quad (5)$$

$$v_{Li} = M_1 / \rho_1 \quad (6)$$

The values of α_1 , β_1 , ξ_1 , and M_1 are input to the program.

2.2.4 Fugacity Ratios

The Redlich-Kwong equation of state is used for calculating vapor properties:

$$P = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)} \quad (7)$$

Equation (7) may be used for either pure component or mixture calculations. For pure components, the parameters are determined from the critical constants:

$$a_1 = R^2 T_{c1}^{2.5} / [9(2^{1/3}-1)P_{c1}] \quad (8)$$

$$b_1 = (2^{1/3}-1)RT_{c1} / (3P_{c1}) \quad (9)$$

The values of P_{c1} and T_{c1} are input to the program. Mixture parameters are determined from pure component parameters and mixture composition:

$$a_m = a_1 x_1^2 + 2\sqrt{a_1 a_2} x_1 x_2 + a_2 x_2^2 \quad (10)$$

$$b_m = b_1 x_1 + b_2 x_2 \quad (11)$$

The fugacity ratio is then calculated from

$$\begin{aligned} \ln \phi_1 = & \left(\frac{Pv}{RT} - 1 \right) b_1 / b_m - \ln [P(v-b_m) / RT] \\ & + \frac{a_m}{b_m RT^{1.5}} \left(2\sqrt{\frac{a_1}{a_m}} - \frac{b_1}{b_m} \right) \ln \left(\frac{v}{v+b_m} \right) \end{aligned} \quad (12)$$

When a pure component fugacity ratio is calculated, $a_m = a_1$ and $b_m = b_1$.

2.2.5 Activity Coefficients

The van Laar equations, modified to allow A_{12} and A_{21} to have opposite signs, are used to calculate activity coefficients as follows:

$$\ln \gamma_1 = A_{12} Z_2^2 (1 - E Z_1) \quad (13)$$

$$\ln \gamma_2 = A_{21} Z_1^2 (1 - E Z_2) \quad (14)$$

where

$$Z_1 = |A_{12}| x_1 / (|A_{12}| x_1 + |A_{21}| x_2) \quad (15)$$

$$Z_2 = 1 - Z_1 \quad (16)$$

and

$$\begin{aligned} E &= 0 && \text{when } A_{12} A_{21} \geq 0 \\ &= 4 && \text{when } A_{12} A_{21} < 0 \end{aligned} \quad (17)$$

The values of A_{12} and A_{21} are the regression parameters for the least squares fit.

3. INPUT

Enter the input data on the blank data sheets of Section 3.1. Numerical data input is in free format and can be punched anywhere on the input card so long as blank spaces separate any two entries. Input data items designated with a double dagger (‡) must be the first item on a new card. The order of punching entries on the card is horizontal, left to right, when two or more columns on the data sheet are not separated by vertical lines, as in list 4. When two columns are separated by double vertical lines (as in list 5), all items in the left hand column are entered before any entries of the right hand column. When successive cases are run, only those input lists different from the preceding case need be included. Each case is terminated by a list 99 card.

3.1 Input Data Forms

PROGRAM 12375, ISOTENISCOPE DATA ANALYSIS INPUT DATA SHEET 1 OF 3

LIST 1: PROBLEM SET IDENTIFICATION and LIST 2: CASE IDENTIFICATION (Optional)	
166	
166	

LIST 3: COMPOSITIONS OF MIXTURES MEASURED		
Item	Description	Entry
2	List Number	± 3
	Number of Mixtures (2 min, 10 max)	±
	Mixture Compositions (Mole Fraction Component 1):	
141-145		
146-150		

LIST 4: TEMPERATURES OF PRESSURE MEASUREMENTS			
Item	Description	Units	Entry
3	List Number		± 4
	Number of Temperature Entries (20 max.)		±
	Temperatures:	°K	
21-25			
26-30			
31-35			
36-40			

± Start New Card

PROGRAM E 1375, ISOTENISCOPE DATA ANALYSIS

Input Data Sheet 2 of 3

LIST 5: PURE COMPONENT PROPERTIES			
Item	Description	Units	Entry
	List Number		† <u>5</u>
	Component Names		Component 1 Component 2
9, 10	Molecular Weight		1 12
21, 22	Antoine Constants	A atm,	
41, 42	($\ln P^* = A + B/(T+C)$)	B °K	
41, 42		C	
11, 12	Critical Temperature	°K	
13, 14	Critical Pressure	atm	
15, 16	Density Coefficients	a g/cm ³ ,	
17, 18	($\rho = a + bT + cT^2$)	b °K	
19, 20		c	

LIST 6: ESTIMATES OF VAN LAAR CONSTANTS (Optional)			
Item	Description	Entry	
	List Number	† <u>6</u>	
	Number of Entries (Temperature Levels, 20 max.)	† <u> </u>	
3	Entry No. (i)	A ₁₂	A ₂₁
	1		
	2		
	3		
	4		
	5		
	6		
	7		
	8		
	9		
	10		

† Start New Card

PROGRAM B1375, ISOTENISCOPE DATA ANALYSIS
Input Data Sheet 2 of 3

LIST 7: MIXTURE ANTOINE CONSTANTS			
Item	Description		Entry
1: 2: 3: 4: 5: 6: 7: 8: 9: 10: A: 22 B: 42 C: 62	List Number		± 7
	Number of Mixture Compositions (10 max)		±
	Mixture Index, i	Antoine Constants A, B, C	
	1	$\ln p^{\circ} = A + B / (T + C)$	
	2	p° = Vapor pressure (atm)	
	3	T = Temperature (°K)	
	4		
	5		
	6		
	7		
	8		

LIST 99: END OF CASE CONTROL

± 99

4. OUTPUT

A typical output printing appears in Section 4.1 following.
Input data used to generate the table are listed in Section 4.2.

4.1 Sample Output

WANNING CYCLE - ANALYSIS OF THERMISTOR DATA
 WFSN 22 PYRAZINE, 5015W
 21375 W 17
 12/ 3/71

COMPONENT	ANTHROPIC CONSTANTS			CRITICAL CONSTANTS			LIQUID DENSITY COEFFICIENTS		
	A	B	C	I (DEG. N)	P (ATM)	A	B	C	
Pyrazine	15.50000	-10615.000	313.520	525.700	60.820	-0.492590	0.005062	-0.1072E-04	
Water	12.03520	-6030.180	-38.150	647.300	218.300	1.047954	-0.000173	0.0	

TEMPERATURE = 300.000 DEG. K., 1000/T = 3.3333 A(1.2) = 4.73889 A(2.1) = 0.57730
 STANDARD DEVIATION = 0.0736ATM

COMPARISON OF EXPERIMENTAL AND CALCULATED PRESSURE

MIXT. NO.	MOL. FRAC. COMP. 1	ANTHROPIC COEFFICIENTS	PRESSURES (ATM)		
			EXP.	CALC.	DIFF.
1	0.25000	14.55300	0.1125	0.0937	-0.0188
2	0.75000	10.78500	0.0644	0.1395	0.0712

TEMPERATURE = 325.000 DEG. K., 1000/T = 3.07692 A(1.2) = 10.00000 A(2.1) = 0.59010
 STANDARD DEVIATION = 0.1060ATM

COMPARISON OF EXPERIMENTAL AND CALCULATED PRESSURE

MIXT. NO.	MOL. FRAC. COMP. 1	ANTHROPIC COEFFICIENTS	PRESSURES (ATM)		
			EXP.	CALC.	DIFF.
1	0.25000	14.55300	0.2946	0.2354	-0.0392
2	0.75000	10.78500	0.2059	0.3033	0.0985

TEMPERATURE = 350.000 DEG. K., 1000/T = 2.85714 A(1.2) = 10.00000 A(2.1) = 0.53377
 STANDARD DEVIATION = 0.1200ATM

COMPARISON OF EXPERIMENTAL AND CALCULATED PRESSURE

MIXT. NO.	MOL. FRAC. COMP. 1	ANTHROPIC COEFFICIENTS	PRESSURES (ATM)		
			EXP.	CALC.	DIFF.
1	0.25000	14.55300	0.6947	0.6447	-0.0502
2	0.75000	10.78500	0.2205	0.6301	0.1096

4.2 Input Data for Section 4.1

FOR THE E1375, ISOTENSIC DATA ANALYSIS

INPUT DATA SHEET 1 OF 3

LIST 1: PROBLEM SET IDENTIFICATION and LIST 2: CASE IDENTIFICATION (Optional)	
RANKINE CYCLE - ANALYSIS OF ISOTENSIC DATA	
MPSN 22 PYRAINE, WATER	

LIST 3: COMPOSITIONS OF MIXTURES MEASURED		
Form	Description	Entry
1	List Number	1
2	Number of Mixtures (2 min, 10 max)	2
Mixture Compositions (Mole Fraction Component 1):		
41-145	0.25 0.75	
1-150		

LIST 4: TEMPERATURES OR PRESSURE MEASUREMENTS			
Form	Description	Units	Entry
1	List Number		1
2	Number of Temperature Entries (20 max)		3
Temperatures:		°K	
41-145	300 325 350		
1-150			
1-150			
1-150			
1-150			

I Start New Card

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PROGRAM C-1375, ISOTHERMSCOPE DATA ANALYSIS

Input Data Sheet 2 of 3

1. PURE COMPONENT PROPERTIES			
Item	Description	Units	Entry
	List Number		# 5
	Component Names		Component 1: PYRAZINE, Component 2: WATER
9.10	Molecular Weight		80.09, 18.016
9.12	Antoine Constant:	A atm,	15.504, 12.0352
9.14	($\ln P^0 = A + B/(T+C)$)	B °K	-10615, -4030.18
9.15		C	313.52, -38.15
9.17	Critical Temperature	°K	625.7, 647.3
9.18	Critical Pressure	atm	66.82, 218.3
9.19	Density Coefficients	a g/cm³,	-0.49259, 1.04794
9.20	($\rho = a + bT + cT^2$)	b °K	.008082, -0.000173
9.21		c	-1.072E-5, 0

2. ESTIMATES OF VAN LAAR CONSTANTS (optional)

Description		Entry	
List Number		# 6	
Number of Entries (Temperature Levels, 20 max.)		I. 3	
Entry No. (i)	Van Laar Constant Estimates	A ₁₂	A ₂₁
1		0.5	0.5
2		0.5	0.5
3		0.5	0.5
4			
5			
6			
7			
8			
9			
10			

* Start New Card

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PROGRAM E1375, ISOTENISCOPIC DATA ANALYSIS

Input Data Sheet 3 of 3

LIST 7: MIXTURE ANTOINE CONSTANTS						
Item	Description		Entry			
	List Number		+ 7			
	Number of Mixture Compositions (10 max)		+ 2			
	Mixture Index, i	Antoine Constants A, B, C	14.553	-6855.7	109.57	
			10.785	-3794.1	-18.29	
	1	$\ln p^{\circ} = A + B / (T + C)$				
	2	p° = Vapor pressure (atm)				
	3	T = Temperature ($^{\circ}\text{K}$)				
	4					
	5					
	6					
	7					
	8					
	9					
	10					
LIST 99: END OF CASE CONTROL						
						79

5. MONSANTO PROPRIETARY SUBROUTINES CALLED

- (1) CDP (with entry points CDP2, CDP3, CDP4)
- (2) HEADER, LINE
- (3) SUMDB
- (4) ERROR
- (5) ZRK
- (6) ZRKCC
- (7) ZRKMC
- (8) LAS

5.1 Function of the Proprietary Subroutines

The call statement followed by a description of the function of each subroutine follows.

```
CALL CDP
CALL CDP2
CALL CDP3
CALL CDP4
```

This subroutine performs the following functions:

- (1) Reading of all list numbers
- (2) Reading and implementation of list 1 and 2
- (3) Implementation of special features such as case incrementing of a specific variable, trial and error solutions, and special summary outputs.

5.2 Call HEADER(KS)

Subroutine HEADER increments a page number counter, prints a two line page heading, and set the line counter in subprogram line to 2. The page heading consists of the list 1 title, program number, and page number on the first line with list 2 title and date on the second line.

The input control code, KS, has the following meanings:

```
KS<0  program number is set from -KS
KS = 0  page number counter is reset to zero
KS = 1  page number counter is incremented by one, page heading
        is written on a new page, and line number counter is
        set at two.
```

Before HEADER is called, the page number counter has a value of zero, hence an initialization call with KS = 0 is not needed. Calling HEADER with KS = 1 assumes that the date and page heading have been stored in the named COMMON section TITL. This function is performed by CDP and the TITL section does not appear in the routine which calls HEADER. If HEADER is not called with KS<0, the program number printed with KS = 1 will be 0000.

5.3 I = LINE(KS)

Function LINE resets, increments, and returns the value of a line number counter. Meaning of the variables follows:

KS	Control code (input) KS<0, LN is set from -KS and stored in LINE KS≥0, LN is incremented by KS and stored in LINE
LINE	Current value of line number counter (output)
LN	Line number counter (internal) at start, LN = 0

5.4 Call SUMDB(DB,I1,I2)

DB(I) Array to be printed (input)
I1 Index of element in array DB where summary starts.
I2 Index of element in array DB where summary ends.

Subroutine SUMDB prints columnwise in four columns the index and value of the non-zero elements of an array.

5.5 Call ERROR(N,NE,LE)

LE(I)	I = 1,NE. Message number list (output)
N	Control code or message number to be added to LE(input) -4≤N≤-1, print message number list N = 0, set NE and LE(I) to zero. N>0, increment NE by 1 and add N to the message number list
NE	Message number counter (output)

Subroutine ERROR initializes an input message list, adds a number to the list, or prints the list according to one of the following formats:

N = 1	CASE SKIPPED DUE TO ERROR IN INPUT ITEM NØ. ____
= 2	CASE SKIPPED DUE TO EXECUTION ERROR NØ. ____
= 3	MODEL EXTRAPOLATED ACCORDING TO MESSAGE NØ. ____
= 4	MODEL EXCEEDED, ASSUMPTIONS MADE, MESSAGE NØ. ____

5.6 Call ZRK(T,P,A,B,Z,KDUM)

T - Absolute temperature (input)
P - Pressure (input)
A - Redlich-Kwong parameter a (input)
B - Redlich-Kwong parameter b (input)
Z - Compressibility factor (output)
KDUM - Dummy variable

Subroutine ZRK calculates the gas compressibility factor by the Redlich-Kwong equation.

5.7 Call ZRKCC(N,TC,PC,ARK,BRK)

N - Number of components (input)
TC(I) - Critical temperatures of components (input)
PC(I) - Critical pressures of components (input)
ARK(I) - Redlich-Kwong a of components (output)
BRK(I) - Redlich-Kwong b of components (output)

Subroutine ZRKCC computes the Redlich-Kwong constants from the critical properties of the components.

5.8 Call ZRKMC(N,Y,ARK,BRK,AM,BM)

N - Number of components (input)
Y(I) - Mole fractions in mixture (input)
ARK(I) - Redlich-Kwong a of components (input)
BRK(I) - Redlich-Kwong b of components (input)
AM - Redlich-Kwong a of mixture (output)
BM - Redlich-Kwong b of mixture (output)

Subroutine ZRKMC calculates mixture Redlich-Kwong constants from mixture composition and pure component Redlich-Kwong constants.

5.9 Call LAS(N,L,A,M,B,X,KERR,KUL,UL,IPS,S,KDET,DET)

N - Number of equations to be solved (input)
L - Number of rows allocated to A,B,UL,X arrays by calling program (input)
A(I,J) - Coefficient matrix of size NxN (input)
M - Control index, set = 1 in present application
B(I) - Vector of right hand sides of equations (input)
X(I) - Solution vector (output)
KERR - Error code (output)
0 normal return,
-1 no solution, A is singular
KUL - Code set to zero in present application

UL(I,J) Scratch matrix, at least NxN
IPS Scratch vector, at least N
S Scratch vector, at least 3N
KDET Code set to zero in present application
DET Value of determinant of A if KDET = 1 (output)

Subroutine LAS solves the linear system of equations $\underline{A} \underline{X} = \underline{B}$
for the vector $\underline{X}$.

6. COMPUTER PROGRAMS (E1375 and RELATED)

```

C  DECLARATIVE SECTION
      COMMON DB(1200), COMP(3,2)
C
C  FILE SECTION
900 FORMAT (G1.0)
901 FORMAT (3A4, G1.0)
C
C  INPUT SECTION
      LNMX = 7
      CALL CDP(DB, LN, LNMX, KTE, KIN)
      CALL HEADER ( -1375)
5  CALL CDP1
      GO TO (11, 5, 13, 14, 15, 16, 17), LN
      IF (LN.EQ. 99) GO TO 30
      CALL EXIT
C  INITIALIZE PROBLEM SET
11 DO 111 I = 1,1200
111  DB(I) = 0.
      DO 112 I = 101, 140
112  DB(I) = 0.5
      GO TO 5
13 READ (5,900) N, (DB(140+I), I=1,N)
      DB(2) = N
      GO TO 5
14 READ (5,900) N, (DB(80+I), I=1,N)
      DB(3) = N
      GO TO 5
15 DO 151 J= 1,2
151 READ (5,901) (COMP(I,J), I=1,3), DB(8+J), DB(20+J), DB(40+J),
      1 DB(60+J), DB(10+J), DB(12+J), DB(14+J), DB(16+J),
      2 DB(18+J)
      GO TO 5
16 READ (5,900) N, (DB(100+I), DB(120+I), I=1,N)
      GO TO 5
17 READ (5,900) N, (DB(22+I), DB(42+I), DB(62+I), I=1,N)
      GO TO 5
C
C  DATA INTERFACE SECTION
C
30 CALL CHECK (NE)
      IF (NE.GT. 0) GO TO 5
C
C  COMPUTATION SECTION
C
40 CALL CDP2
50 CALL MODEL
      CALL CDP3
      IF (KTE.GT. 0) GO TO 50
C
C  OUTPUT SECTION
      IF (DB(5).NE. 1.) CALL OUTPUT
      CALL CDP4
      IF (KIN.EQ. 1) GO TO 40
      GO TO 5
      END

```

```

SUBROUTINE GAMMA (A, X, G1, G2, Z1, Z2)
DIMENSION A(2)
      Z1 = A(1)*X/(A(1)*X+A(2)*(1.-X))
      Z2 = 1. - Z1
      G1 = EXP(A(1)*Z2**2)
      G2 = EXP(A(2)*Z1**2)
RETURN
END

```


SUBROUTINE CHECK (NE)

C

C

DECLARATIVE SECTION

COMMON DB (1200)

DIMENSION LE (20)

C

C

COMPUTATION SECTION

CALL ERROR (0, NE, LE)

IF (DB(2) .LT. 1.)

IF (DB(3) .LT. 1.)

IF (DB(9) .LE. 1.)

IF (DB(10) .LE. 1.)

CALL ERROR(1, NE, LE)

CALL ERROR(2, NE, LE)

CALL ERROR(9, NE, LE)

CALL ERROR(10, NE, LE)

DO 10 I = 1, 12
10 IF (DB(40+I) .GT. 0.0)

CALL ERROR (40+I, NE, LE)

DO 20 I = 1, 4
20 IF (DB(10+I) .LE. 0.)

CALL ERROR (10+I, NE, LE)

IF (DB(5) .LT. 2. .AND. NE .LE. 0) GO TO 30

CALL HEADER(1)

CALL SUMDB (DB, 1, 1200)

30 IF (NE .GT. 0) CALL ERROR (-1, NE, LE)

RETURN

END

```

SUBROUTINE MODEL
C
C      SUBROUTINE TO CALCULATE VAN LAAR CONSTANTS FROM ISOTENISCUE
C      VAPOR PRESSURE MEASUREMENTS.
C
C  DECLARATIVE SECTION
COMMON      DH(1200)
DIMENSION  AA(2),      AR(2),      AC(2),      AAM(10),
1          ABM(10),     ACM(10),     AD(2),      HD(2),      CD(2),
2          A12S(20),    A21S(20),    T(20),      TC(2),      PC(2),
3          WM(2),       STDEV(20),    DQDA(2),     D2QDA(2,2),    A(2,20),
4          POYNT(2,10), PHIL(2,10),  PHIV(2,10),  TREC(10),    DP1DA(2,10),
5          P1(10),      P2(10),      DP1(2,10),  DP2(2,10),  USEP1(2,2),
6          10), DSECP2(2,2,10), P(10,20), PCAL(10,20), DP(10,20),
7          FLP(2,10),   PPR(2,10),   VPRESS(2),   TCX(1,2),   FLPx(2),
8          ARK(2),      BRK(2),      TPS(2),      UL(2,2),    S(6),
          DIMENSION  ABEST(2),  ASTART(2),  XUB(2),    ALB(2),
1          DATA(3),  NDATA(8),  DELA(2),    U(3),
2          X(10)
C  INTERFACE SECTION
C
EQUIVALENCE (AA,DB(21)),      (AB,DB(41)),      (AC,DB(61)),
1          (AAM,DB(23)),      (ABM,DB(63)),      (ACM,DB(67)),
2          (A12S,DB(101)),    (A21S,DB(121)),    (T,DB(81)),
3          (TC,DB(11)),      (PC,DB(13)),      (WM,DB(9)),
4          (STDEV,DB(161)),   (DQDA,DB(153)), (D2QDA,DB(155)),
5          (A,DB(201)),      (POYNT,DB(241)), (PHIL,DB(261)),
6          (PHIV,DB(281)),   (TREC,DB(321)), (DP1DA,DB(341)),
7          (DP2DA,DB(361)),  (DP1DA,DB(381)), (DP2DA,DB(421)),
8          (P,DB(501)),      (PCAL,DB(701)), (DP,DB(901)),
9          (FLP,DB(461)),    (PPR,DB(301)), (VPRESS,DB(181))
EQUIVALENCE (TCX,DB(481)),   (X,DB(141))
C
C      NMIX = DB(2)
C      NTEMP = DB(3)
CALL ZRKCC(2, TC, PC, ARK, BRK)
C  COMPUTATION SECTION
C
DO 10 I = 1, NTEMP
10  TREC(I) = 1000./T(I)
DO 11 I = 1, 2
11  TCX(I) = TC(I)
DO 12 I = 3, 12
12  TCX(I) = 1000.
C
C  - - - - - ESTABLISH TEMPERATURE LEVELS
C
DO 100 I = 1, NTEMP
K = NMIX + I
DO 20 J = 1, 2
20  VPRESS(J) = VP(T(I),J)
DO 22 J = 3, K
22  P(J-2,I) = VP(T(I),J)
DO 22 L = 1, 4
22  FLP(L,J-2) = VPRESS(L)/P(J-2,I)
C  - - - - - FUGACITY AND POYNTING CORRECTIONS

```

```

C
DO 30 J = 1, NMIX
CALL RKWONG(2,T(I),P(J,I),PHIL(1,J),PHIV(1,J),FLP(1,J),ARK,BRK)
30 CALL PUFCOR(2, T(I), P(J,I),POYNT(1,J), FLP(1,J))
C
C - - - - - STARTING VALUES FOR A
A(1,1) = A12S(I)
40 A(2,1) = A21S(I)
C
C - - - - - INITIATE SEARCH
NDATA(1) = 1
NDATA(6) = 100
NDATA(7) = 1000
DATA(2) = 0.1
DATA(3) = .0001
DO 41 K = 1, 2
XUB(K) = 10.
XLR(K) = .00001
41 CALL SRCH(3,A(1,1), ABEST, ALAST, XUB, XLB, DQDA, D2QDA, 2,
DATA, NDATA, DELX, IPS, S, UL)
1 IF (NDATA(1) .LE. 0) GO TO 90
Q(1) = 0.
DO 60 J = 1, NMIX
CALL GAMMA (A(1,1), X(J), G1, G2,Z1,Z2)
P1(J) = G1*VPRESS(1)*PHIL(1,J)*POYNT(1,J)*X(J)/PHIV(1,J)
P2(J) = G2*VPRESS(2)*PHIL(2,J)*POYNT(2,J)*(1.-X(J))/
PHIV(2,J)
1 PCAL(J,1) = P1(J) + P2(J)
Q(1) = Q(1) + (P(J,1) - PCAL(J,1))**2
IF (NDATA(1) .EQ. 2) GO TO 60
DP1(1,J) = P1(J)*Z2**2*(1.-2.*Z1)
DP1(2,J) = 2.*P1(J)*Z1*Z2**2*A(1,1)/A(2,1)
DP2(1,J) = 2.*P2(J)*Z2*Z1**2*A(2,1)/A(1,1)
DP2(2,J) = P2(J)*Z1**2*(1.-2.*Z2)
DSECP1(1,1,J) = P1(J)*Z2**2*(Z2**2*(1.-2.*Z1)**2-2.*(2.*Z2-Z1)
* Z1/A(1,1))
DSECP1(1,2,J) = 2.*P1(J)*Z1*Z2**2*(A(1,1)*Z2**2*(1.-2.*Z1) +
2.*Z2-Z1)/A(2,1)
1 DSECP1(2,1,J) = DSECP1(1,2,J)
DSECP1(2,2,J) = 2.*P1(J)*Z1*Z2**2*A(1,1)*(2.*A(1,1)*Z1*Z2**2
+1.-3.*Z2)/A(2,1)**2
1 DSECP2(1,1,J) = 2.*P2(J)*Z2*Z1**2*A(2,1)*(2.*A(2,1)*Z2*Z1**2 +
1.-3.*Z1)/A(1,1)**2
1 DSECP2(1,2,J) = 2.*P2(J)*Z1**2*Z2*(A(2,1)*Z1**2*(1.-2.*Z2)
+2.*Z1-Z2)/A(1,1)
1 DSECP2(2,1,J) = DSECP2(1,2,J)
DSECP2(2,2,J) = P2(J)*Z1**2*(Z1**2*(1.-2.*Z2)**2-2.*Z2*
(2.*Z1-Z2)/A(2,1))
1
60 CONTINUE
IF (NDATA(1) .EQ. 2) GO TO 50
DO 65 J = 1, 2
DQDA(J) = 0.
DO 65 K = 1, NMIX
65 DQDA(J) = DQDA(J) + 2.*(PCAL(K,1)-P(K,1))*(DP1(J,K)+DP2(J,K))
1
D2QDA(1,1) = 0.
D2QDA(1,2) = 0.
D2QDA(2,2) = 0.

```

```

      NO 70 J = 1, NMIX
          D2QDA(1,2) = D2QDA(1,2) + 2.*((PCAL(J,I)-P(J,I))*(DSECP1
1          (1,2,J)+DSECP2(1,2,J))*(DP1(1,J)+DP2(1,J))*
2          (DP1(2,J)+DP2(2,J)))
      NO 70 K = 1,2
70      D2QDA(K,K) = D2QDA(K,K) + 2.*((DP1(K,J)+DP2(K,J))*((
1          (PCAL(J,I)-P(J,I))*(DSECP1(K,K,J)+
2          DSECP2(K,K,J)))
          D2QDA(2,1) = D2QDA(1,2)
      GO TO 50
90 NO 91 J = 1, NMIX
91      DP(J,I) = PCAL(J,I) - P(J,I)
          STDEV(I) = SQRT(Q(1)/FLOAT(NMIX-1))
100 CONTINUE
      RETURN
      END

```

```

SUBROUTINE OUTPUT
C
C DECLARATIVE SECTION
COMMON DB(1200), COMP(3,2)
C
C FILE SECTION
1000 FORMAT (1H0, COMPONENT, ' MOLECULAR - - - ANTOINE
1 CONSTANTS - - - - CRITICAL CONSTANTS - - LIQUID DENSITY C
2 COEFFICIENTS' / 18X, 'WEIGHT' 6X,
3 'A' 11X, 'B' 11X, 'C' 7X, 'T (DEG. K) P (ATM)' 6X,
4 'A' 11X, 'B' 11X, 'C')
1001 FORMAT (1X, 3A4, F11.3, F12.5, 4F12.3, 2F12.6, G12.4)
1002 FORMAT (1H0, 'TEMPERATURE =' F9.3, 'DEG. K., 1000/T =' F12.4, 2X
1 'A(1,2) =' F9.5, 2X 'A(2,1) =' F9.5)
1004 FORMAT (1X, 'STANDARD DEVIATION =' F10.4, 'ATM')
1005 FORMAT (1H0, 'COMPARISON OF EXPERIMENTAL AND CALCULATED PRESSURE')
1006 FORMAT (1H0, 'MIXT. MOLE FRAC ANTOINE COEFFICIENTS' 16X,
1 - - - - PRESSURES (ATM) - - - / ' NO. COMP. 1 A
2 B C EXP. CALC. DIFF. ')
1007 FORMAT (16, 2F12.5, 5F12.4)
C
C DATA INTERFACE SECTION
NM = DB(2)
NT = DB(3)
C
C OUTPUT SECTION
IK = 1
10 CALL HEADER (1)
WRITE (6, 1000)
DO 11 I = 1, 2
11 WRITE (6, 1001) (COMP(K,I), K=1,3), DB(8+I), DB(20+I), DB(40+I),
1 DB(60+I), DB(10+I), DB(12+I), DB(14+I), DB(16+I),
2 DB(18+I)
C
20 WRITE (6, 1002) DB(80+IK), DB(320+IK), (DB(200+2*(IK-1)+I), I=1,2)
WRITE (6, 1004) DB(160+IK)
WRITE (6, 1005)
WRITE (6, 1006)
DO 25 I = 1, NM
25 WRITE (6, 1007) I, DB(140+I), DB(22+I), DB(42+I),
1 DB(62+I), DB(500 + I + 10*(IK-1)), DB(700 + I + 10*(IK-1)),
2 DB(900 + I + 10*(IK-1))
IK = IK + 1
IF (IK .GT. NT) RETURN
IF (IK .EQ. 4 .OR. IK .EQ. 7 .OR. IK .EQ. 10) GO TO 10
GO TO 20
END

```

```

SUBROUTINE POYCOR( N, TA, PATH, POYNT, FLP)
DATA R / 82.0575 /
COMMON DB (1200)
DIMENSION      ALD(1),      BLD(1),      CLD(1),      WM(1),
1      TC(1),      POYNT(1),      FLP(1)
EQUIVALENCE (DB(9),WM),      (DB(15),ALD),      (DB(17),BLD),
1      (DB(19),CLD),      (DB(1),TC)
DO 20 I
      = 1+N
IF      (ALD(I) .EQ. 0.) GO TO 10
C      V=LIQ VOLUME IN CC/GMOL
      V      = WM(I)/(ALD(I)+TA*(BLD(I)+TA*CLD(I)))
      PVP      = FLP(I)*PATH
IF      (TC(I) .GT. 0. .AND. TA .GT. TC(I)) PVP = 1.
      E      = V*(PATH-PVP)/(R*TA)
IF      (E .GT. 100.) CALL TERNIN(4,I,TA)
      POYNT(I) = EXP(E)
GO TO 20
10      POYNT(I) = 1.
20 CONTINUE
RETURN
END

```


RETURN
END

```

SUBROUTINE SRCH(Q,X,X1,X2,XUB,XLB,DQDX,D2QDX,NX,DATA,NDATA,DELX,
1      IPS,S,UL)
C      THIS SUBROUTINE HAS AS ITS PURPOSE A SEARCH FOR A SET OF
C      PARAMETERS, X, WHICH MINIMIZES A FUNCTION Q. VALUES OF THE
C      FUNCTION AND ITS DERIVATIVES ARE TO BE SUPPLIED BY THE CALLING
C      PROGRAM WHEN REQUESTED BY SRCH.
C
C      * * * * * DEFINITION OF VARIABLES * * * * *
C
C      Q      ARRAY OF Q VALUES. Q(1) = VALUE IN CURRENT CALCULATION
C              Q(2) = BEST VALUE
C              Q(3) = FIRST VALUE AT PRESENT STEP
C              SIZE
C
C      X      VECTOR OF PARAMETERS WHICH DETERMINE Q.
C      X1     BEST SET OF X VALUES
C      X2     X VALUES AT START OF PRESENT STEP SIZE.
C      XUB    UPPER BOUNDS ON X VECTOR
C      XLB    LOWER BOUNDS ON X VECTOR
C      DQDX   VECTOR OF FIRST DERIVATIVES OF Q
C      D2QDX  MATRIX OF SECOND DERIVATIVES OF Q
C      NX     DIMENSION OF X VECTOR
C      DATA  REAL DATA ARRAY FOR SUBROUTINE
C      NDATA  INTEGER DATA ARRAY FOR SUBROUTINE
C      ITER   NUMBER OF ITERATIONS, INCLUDING DERIVATIVES, IN SEARCH
C      ICODE  STATUS CODE FOR COMPUTATIONS
C              1 = FIRST CALL OF SRCH
C              2 = CALL FOR COMPUTATION OF Q
C              3 = CALL FOR COMPUTATION OF Q AND ITS FIRST
C                AND SECOND DERIVATIVES
C              0 = CONVERGED SOLUTION
C              -1 = NOT CONVERGED, BUT MINIMUM STEP SIZE REACHED
C              -2 = NOT CONVERGED, MAXIMUM ITERATIONS EXCEEDED
C              -3 = NOT CONVERGED, MAXIMUM FUNCTIONAL
C                EVALUATIONS EXCEEDED
C
C      NFE    NUMBER OF FUNCTIONAL EVALUATIONS
C      EPS    CONVERSION CRITERION ON DERIVATIVES
C      STEPSD STEEPEST DESCENT STEP SIZE
C      STEPNR NEWTON RAPHSON STEP SIZE
C      ITERA  NUMBER OF ITERATIONS AT CURRENT STEP SIZE
C      MODE   METHOD OF INCREMENTING X
C              1 = NEWTON-RAPHSON
C              2 = STEEPEST DESCENT
C
C      MXITER MAXIMUM NUMBER OF ITERATIONS ALLOWED
C      MAXFE  MAXIMUM NUMBER OF FUNCTIONAL EVALUATIONS ALLOWED
C
C      DECLARATIVE SECTION
C
C      DIMENSION DELX(1), IPS(1), S(1), UL(NX,1)
C      DIMENSION Q(3), X(1), X1(1), X2(1), XUB(1),
1      XLB(1), DQDX(1), D2QDX(NX,1), DATA(3), NDATA(8)
C
C      INTERFACE SECTION
C
C      EPS = DATA(1)
C      IF (EPS .LE. 0.) EPS = 0.0001
C      STEPSD = DATA(2)
C      STEPNR = DATA(3)

```

```

      ICODE = NDATA(1)
      ITER = NDATA(2)
      NFE = NDATA(3)
      ITERA = NDATA(4)
      MODE = NDATA(5)
      MXITER = NDATA(6)
      MAXFE = NDATA(7)
      NVAR = NDATA(8)

C
C  COMPUTATION SECTION
C
      IF (ICODE .NE. 1) GO TO 200
C
C  - - - - - INITIATE SEARCH
100      ITER = 0
          ICODE = 3
          NFE = 0
          ITERA = 0
          GO TO 700
C
C  - - - - - TEST FOR TOO MANY EVALUATIONS
200      NFE = NFE + 1
          IF (NFE .LT. MAXFE) GO TO 400
C
C  - - - - - ERROR RETURN
300      ICODE = -3
301 DO 302 I = 1,NX
302      X(I) = X1(I)
          Q(1) = Q(2)
          GO TO 700
C
C  - - - - - TEST ICODE
400 IF (ICODE .NE. 2) GO TO 600
C
C  - - - - - TEST FOR REDUCTION IN Q
500 IF (Q(1) .LT. Q(2)) GO TO 570
510 IF (MODE .EQ. 2) GO TO 530
520      MODE = 2
          GO TO 545
C
C  - - - - - STEP SIZE REDUCTION
530 IF (ITERA .GE. 10) GO TO 565
          STEPSD = 0.25*STEPSD
          IF (STEPSD .LT. EPS) GO TO 560
540      ITERA = 0
C
C  - - - - - STEEPEST DESCENT CALCULATION
545      SUM = 0.
          DO 546 I = 1,NX
546      SUM = SUM + DQDX(I)**2
          DO 547 I = 1, NX
              X(I) = X1(I) - STEPSD*DQDX(I)/SQRT(SUM)
              IF (X(I) .LT. XLB(I)) X(I) = XLB(I)
              IF (X(I) .GT. XUB(I)) X(I) = XUB(I)
547 CONTINUE
          GO TO 700
560      ICODE = -1
          GO TO 301

```

```

C - - - - - RETURN FROM ACCELERATED VECTOR
C 565      ICODE = 3
          ITERA = 0
          GO TO 301

C - - - - - SMALLER OBJECTIVE FUNCTION FOUND
C 570 DO 571 I = 1,NX
571      X1(I) = X(I)
          Q(2) = Q(1)
          IF (ITERA .GE. 10) GO TO 590
580      ITERA = ITERA + 1
          ICODE = 3
          GO TO 700

C - - - - - COMPUTE ACCELERATED VECTOR
C 590 DO 591 I = 1,NX
          X(I) = 2.*X1(I)-X2(I)
          IF (X(I) .LT. XLB(I)) X(I) = XLB(I)
          IF (X(I) .GT. XUB(I)) X(I) = XUB(I)
591 CONTINUE
          GO TO 700

C - - - - - INITIATE NEW ITERATION
C - - - - - CONVERGENCE TEST
600      B = 0.
          DO 601 I = 1, NX
          IF (B .LT. ABS(DQDX(I))) B = ABS(DQDX(I))
601 CONTINUE
          IF (B .GT. 0.001*EPS) GO TO 620
610      ICODE = 0
          GO TO 700

C - - - - - TEST FOR EXCESS ITERATIONS
C 620 IF (ITER .LT. MXITER) GO TO 640
630      ICODE = -2
          GO TO 301

C - - - - - NEWTON RAPHSON SEARCH
C 640      MODE = 1
          DO 641 I = 1, NX
          X1(I) = X(I)
          IF (ITERA .EQ. 0) X2(I) = X(I)
641 CONTINUE
          Q(2) = Q(1)
          IF (ITERA .EQ. 0) Q(3) = Q(1)
          ITER = ITER + 1
          DO 642 I = 1,NX
          DQDX(I) = -DQDX(I)
          CALL LAS(NX,NX,D2QDX,1,DQDX,DELX,KERR,0,UL,IPS,S,0,DET)
          DO 643 I = 1,NX
          DQDX(I) = -DQDX(I)
          IF (KERR .NE. 0) GO TO 690
          DO 644 I = 1,NX
          X(I) = X1(I) + DELX(I)
          IF (X(I) .GT. XUB(I)) X(I) = XUB(I)
          IF (X(I) .LT. XLB(I)) X(I) = XLB(I)
644 CONTINUE

```

```

        ICODE = 2
GO TO 700
690    ICODE = -10 + KERR
C
C - - - - - RETURN INTERFACE SECTION
700    DATA(2) = STEPSD
        NDATA(1) = ICODE
        NDATA(2) = ITER
        NDATA(3) = NFE
        NDATA(4) = ITERA
        NDATA(5) = MODE
RETURN
END

```



```

SUBROUTINE TERMIN ( NUM, NCOMP, BAD )
C
COMMON DB(1)
WRITE (6,100)
100 FORMAT( 'FATAL ERROR HAS OCCURRED DURING COMPUTATION...' )
GO TO (1,2,3,4,5,6,7,8,9,10), NUM
GO TO 99
1 CONTINUE
WRITE (6,101) NCOMP, BAD
101 FORMAT(//, 'LOG(E) OF VAPOR PRESSURE FOR COMPONENT',I3,
1 ' EXCEEDS 100. AT TEMPERATURE',1PG15.4, ' DEG K' )
GO TO 99
2 CONTINUE
WRITE (6,102) NCOMP, BAD
102 FORMAT(//, 'LOG(E) OF PRAUSNITZ-SHAIR (COMPON',I3,') EXCEEDS 100.'
1 ' AT TEMPERATURE',1PG15.4, ' DEG K' )
GO TO 99
3 CONTINUE
WRITE (6,103) NCOMP,BAD
103 FORMAT(//, 'LOG(E) OF ACTIVITY COEFF (VAN LAAR) EXCEEDS 100.'
1 ' FOR COMPONENT',I3, ' AT T =',1PG12.4, ' DEG K.' )
GO TO 99
4 CONTINUE
WRITE (6,104) NCOMP, BAD
104 FORMAT(//, 'LOG(E) OF POYNTING CORRECTION FOR COMPONENT',
1 ' I3, EXCEEDS 100. AT TEMPERATURE',1PG15.4, ' DEG K',
2 //, ' CHECK LIQUID DENSITY DATA AND/OR UNITS' )
GO TO 99
5 CONTINUE
WRITE (6,105) NCOMP, BAD
105 FORMAT( '0', ' FAILURE IN ATTEMPT TO COMPUTE COMPRESSIBILITY',
1 ' FACTOR FOR COMPONENT',I3, ' AT TEMPERATURE',
2 ' 1PG12.4, DEG, K, // NO VALUE FOR Z WAS FOUND',
3 ' BETWEEN 0 AND 4, CHECK CRITICAL PROPERTIES',
4 ' FOR THIS COMPONENT' )
GO TO 99
6 CONTINUE
WRITE (6,106) NCOMP, BAD
106 FORMAT( '0', ' FAILURE TO COMPUTE FUGACITY COEFFICIENT FOR',
1 ' COMPONENT',I3, ' AT',1PG12.4, ' DEG K',
2 //, ' CHECK CRITICAL PROPERTY DATA' )
GO TO 99
7 CONTINUE
WRITE (6,107) NCOMP, BAD
107 FORMAT( '0', ' LOG( A(I,J) ) EXCEEDS 100. FOR THE WILSON FORM',
1 ' (COMP. NO., I3, )',
2 ' AT TEMPERATURE',1PG15.7, ' K. ' )
GO TO 99
8 CONTINUE
WRITE (6,108) BAD
108 FORMAT( '0', ' FAILURE TO COMPUTE A(I,J) FROM INF. DIL. ACT. COEF',
1 ' F. (WILSON FORM) HAVING A VALUE OF',1PG15.6,
2 ' CHECK HENRY'S LAW CONSTANTS' )
GO TO 99
9 CONTINUE
GO TO 99
10 CONTINUE

```

GO TO 99
99 CALL SUMDB (DB: 1.1200)
WRITE (6,200)
200 FORMAT(/////0***** UNABLE TO PROCEED. ENTIRE JOB ABORTED *****)
CALL EXIT
RETURN
END

```

FUNCTION VP ( T, I )
COMMON DB(1200)
DIMENSION AA(1), AB(1), AC(1), WM(1),
1 TC(1), PC(1)
EQUIVALENCE (DB(2),AA), (DB(4),AB), (DB(6),AC),
1 (DB(9),WM), (DB(48),TC), (DB(13),PC)
KPHI = 0
C CHECK IF COMPONENT ABOVE CRITICAL
IF (KPHI .EQ. 1 .AND. TC(I) .GT. 0. .AND. T .GT. TC(I))
1 GO TO 100
C USE PRAUSNITZ-SHAIR BELOW CRITICAL
C IF ANTOINE CONSTANTS WERE NOT GIVEN.
IF (AA(I) .EQ. 0.) GO TO 100
C BELOW CRITICAL. USE ANTOINE
A = AA(I)
B = AB(I)
C = AC(I)
C ANTOINE EQ. CONTAINS SINGULAR POINT AT
C VERY LOW TEMPERATURES ( T = - C). THE
C FOLLOWING CODE PREVENTS SINGULARITY AND
C VAPOR PRESSURE REVERSAL AT T LESS THAN -C
D = T + C
IF (D .GT. 10.) GO TO 50
A = A + B*C/100.
B = B*(1. - C/10.)*2
D = T
50 E = A + B/D
C ERROR IF VAPOR PRESSURE EXCEEDS 1.E+3
IF (E .GT. 100.) CALL TERMIN( 1, I, T )
VPTM = EXP(E)
C SET LOWER LIMIT ON VAPOR PRESSURE
C FOR HEAVY COMPONENTS AT LOW TEMPERATURES
VP = AMAX1(VPTM,1.E-30)
GO TO 500
C HYPOTHETICAL LIQUID FUGACITY FROM
C PRAUSNITZ-SHAIR
100 IF (WM(I) .GT. 5.) GO TO 150
C HYDROGEN AND HELIUM
E = 6.495 + .2388/(T-277.783) - 3.8394E-3*(T-273.15)
IF (E .GT. 100.) CALL TERMIN(2, I, T)
VP = EXP(E)
GO TO 500
C ALL OTHER COMPONENTS
150 TR = T/TC(I)
E = 6.088 - 5.109/(TR - .0971) - .8282*TR
IF (E .GT. 100.) CALL TERMIN(2, I, T)
VP = PC(I)*EXP(E)
500 CONTINUE
RETURN
END

```

APPENDIX M

TEMPERATURE-ENTROPY DIAGRAM PLOTTING Computer Program TSPLIT

1. DESCRIPTION

1.1 Scope

TSPLIT uses data from Program E1393 to produce a thermodynamic plot. The plot consists of:

- (a) a title
- (b) labeled axes (Y-axis is temperature; X-axis is entropy)
- (c) a curve which defines the boundary of the two-phase region
- (d) contours at selected values for up to three functions (Pressure, Density, or Enthalpy). Contours are identified with labels.

1.2 Model

Values of the functions are generated at each point of a temperature-pressure grid in Program E1393. TSPLIT locates coordinates for points along a requested contour. The contour is plotted according to rules specific to the particular function. Actual plotting is done using Calcomp routines (ref. 1), or modifications of them (section 5).

1.3 Limitations

TSPLIT expects the function data to be located in COMMON exactly as defined in Program E1393.

The maximum lengths of the X and Y axes are 100 and 25 inches, respectively. However, a practical limit for X of about 2" to 30 inches should be assumed to avoid exceeding the size of certain arrays.

The number of requested contour levels should not exceed 100 for each function.

2. SUBPROGRAM USAGE

2.1 General

Only two statements were added to Program E1393 to permit it to use TSPLIT. A "CALL TSPLIT" was required after E1393 has completed its output but before it returns to statement 5 to read the control list. The other statement needed was a "CALL GRAPHE" just before the "CALL EXIT" in E1393.

TSPLIT contains its own READ statements. Instructions for punching cards for input to TSPLIT are given in section 2.2. Output from TSPLIT to the printer is explained in section 2.3.

2.2 Input

2.2.1 Cards Required by TSPLIT (see section 6 for formats)

Each new thermodynamic diagram requires the four cards described below plus as many cards as needed to request the desired contours.

Card 1: Columns 1 through 72 may contain any character
(TITLE) desired in the title. The title is drawn starting at the top left of the plot.

Card 2: Columns 1 through 36 contain any desired characters
(AXISID) for labeling the X-axis. Columns 37 through 72 are used for the X-axis label.

Card 3: This card must contain six numbers, separated by
(SCALES) at least one blank. The first three numbers specify: X-axis length in inches; minimum X-value for labeling X-axis, and maximum X-value for the X-axis. The fourth through sixth numbers specify the corresponding information for the Y-axis.

Card 4: Only one number is to be punched on this card.
(IDBUG) Normally, a zero punch will be used (in any column). Any number other than zero will cause a detailed printout of arrays and other data from TSPLIT.

Two, or more, additional cards are required to define which function and what contour values are to be plotted. The first of these cards (KONTUR) must contain only one number to identify the function. Valid function numbers are:

- 1 (pressure)
- 2 (density)
- 3 (enthalpy)

If the number punched is less than 1, TSPLIT will return to program E1393. If it is greater than 3, the program will terminate. The plotting of a thermodynamic diagram should normally be terminated by using the above card with a number less than one.

When function 1, 2, or 3 is indicated, the above card must be followed with a card(s) specifying how many contours are requested and what is the level (value) for each of these contours. As many cards are needed may be used to specify contour levels. Numbers on the cards must be separated by at least one blank.

Section 6 contains a form which can be used to prepare input cards for TSPLIT.

2.2.2 Placement of Cards in Input Deck

Program E1393 requires its own input cards. For each case run in E1393 the last card is punched with only the number 99 on it. The deck of TSPLIT cards for that case should follow the "99" card. This sequence is repeated for each case to be plotted.

2.2.3 Suggestions for Selecting Values for Card 3 (SCALES)

The six numbers on this card provide scaling information to TSPLIT. For each axis the value of (maximum-minimum)/length determines the units per inch along that axis. If necessary, adjust any of the three values to obtain a convenient number for units per inch. Make a final adjustment to the maximum value and length, if needed, so that maximum at least equals the actual data maximum plus $2 * (\text{units per inch})$. In any event, the final adjusted maximum and minimum values must span the true data maximum and minimum.

2.2.4 Selecting Values for Pressure Contours

Although the raw data from program E1393 is given on a pressure grid, pressure contours may be requested for any pressure level within the extremes provided by E1393. To assure that full contours can be plotted for those extreme values, the input to E1393 (List 4) should include one pressure slightly below the lowest contour desired and one slightly above the highest contour desired. Suggested values are approximately $1.005 * \text{maximum contour level}$ and $0.995 * \text{minimum contour}$.

2.3 Output

In addition to the plot described in 1.1, TSPLIT will output the following to the printer.

1. title card data
2. axes labels card data
3. scaling data (from card 3)
4. number of temperature and pressure values in the base grid
5. identification of the contour levels plotted for each function.

If card 4 was punched with something other than a zero, a detailed debugging printout will be obtained.

Three error codes and one error message can be printed:

ERROR CODE

MEANING

- | | |
|---------|--|
| 1 | Less than 3 points remain on boundary. |
| 3 and 4 | An invalid function number was used. |

The error message indicates that too many points were generated when densifying the data. The message is:

"FLINE - IK TOO BIG"

3. EXAMPLE

Section 6 shows input cards for TSPLIT, printed output from TSPLIT, and a reduced copy of the diagram.

4. REFERENCES

1. Bulletin titled "Programmin CalComp Pen Plotters" and a manual titled "CalComp Graphics Functional Software, USAS Fortran Scientific" both from California Computer Products, Inc., Anaheim, California.
2. Monsanto Technical Subprogram Manual, program GRAPHE.
3. Documentation for program El393.

5. PROCEDURE USED IN TSPLIT

5.1 Introduction

Program El393 produces four arrays of data used in TSPLIT. These arrays are in blank COMMON and are named:

PG	a one-dimensional array of grid pressures
TG	a one-dimensional array of grid temperatures
RE	a two-dimensional array of data on the two phase boundary
RG	a three-dimensional array of data for the single phase regions

After all thermodynamic data has been stored in these arrays, E1393 calls TSPL0T. TSPL0T reads four cards of input (section 2.2.1) and then draws the axes, a border, and the title. Additional cards are read defining the contours and valid contour levels are then plotted.

5.2 Subroutine FLINE

FLINE is a Calcomp subroutine (ref. 1) which uses a modified spline technique to place a smooth curve through a given set of points and plot the curve. It has been altered to save and return arrays containing the coordinates for the smooth curve. Since those coordinates are spaced sufficiently close for plotting, FLINE, in effect, "densifies" the given data. With closely spaced points, linear interpolation is adequate to determine coordinate values between the points generated by FLINE. An option is provided in the modified FLINE so that it can be used to plot the smooth curve or not. In either case the dense set of coordinates are returned to the calling program. FLINE is used both ways in TSPL0T.

5.3 The Two-Phase Boundary

Temperature-Entropy coordinates along the two-phase boundary are extracted from array RE. Those points are available in pairs at the same temperature: one on the liquid side and one on the gas side of the boundary. The liquid side data is scanned in the direction of increasing temperature. A liquid side boundary point is deleted if its entropy is less than the entropy at the preceding lower temperature. This step is required to minimize certain problems which sometimes occur with data near the critical temperature.

The boundary is plotted in two parts: the liquid side and the gas side. A straight line is drawn connecting the two sides at the highest temperature for which boundary data is given unless that data was deleted. FLINE is used to plot the boundary. The dense set of boundary coordinates is saved by TSPL0T.

5.4 Contours

TSPL0T next reads a card to identify which function (Pressure, Density, or Enthalpy) is to be plotted. It then reads a card(s) which specifies the number of contours requested and their values.

Data for the function along the two phase boundary is extracted from array RE. FLINE is again used to get a dense set of temperature-function values along the boundary. This boundary data is used to locate any intersections of a contour with the boundary.

Each requested contour value is processed as follows. A test is made to determine if the requested contour level is acceptable. All values for pressure contours are accepted. A Density contour is rejected if it is greater than the density of the highest temperature on the gas side of the boundary. An Enthalp contour is rejected if it is less than the enthalpy at the lowest temperature on the gas side of the boundary. However, if an enthalpy contour intersects the liquid side of the boundary, a tic mark is drawn at the boundary intersection. Except for Pressure, no contours are drawn through the two phase region.

5.4.1 Coordinates for Pressure Contours

Points along a pressure contour are found from the data grid as follows. For each grid temperature all the entropy data for all grid pressures are extracted from array RG. If there are intersections with the boundary, each side of the boundary is handled separately. This array of entropies and an array of corresponding pressures are saved by TSPLIT. If the array of pressures spans the requested contour value, the pair of arrays is densified using FLINE. The required entropy value is found by linear interpolation from the dense data. This entropy and its corresponding temperature define one point on the contour.

After locating all such points, FLINE is used to plot the contour. If the pressure contour passes through the boundary region, a straight line is drawn connecting the points of intersection with the boundary. In this case the contour value is labeled along the straight line segment. Otherwise, the value is labeled along the high temperature end of the contour.

5.4.2 Coordinates for Density Contours

A similar procedure is used to locate points for a Density contour. No lines are drawn through the boundary region, however, and dashed lines are plotted for these contours. Labels are placed above the high temperature ends of the contours.

5.4.3 Coordinates for Enthalpy Contours

In addition to locating coordinates in the same way as for Density, the data grid is scanned for all temperatures at each given pressure. This step is necessary for Enthalpies because, at high entropies, the contours may nearly parallel the entropy axis.

Labels for enthalpy contours are placed at the high entropy end of the curve. On the liquid side of the two phase region, tic marks are drawn and labeled at intersections with the boundary.

5.5 Termination

When TSPLIT reads a card identifying a function with a number less than 1, it returns to Program E1393. E1393 may generate another case and call TSPLIT again. If no more cases are run, E1393 executes a CALL GRAPHE before ending execution.

If any of the errors detected by TSPLIT occur, TSPLIT will CALL GRAPHE, then stop execution. Some run-time errors, such as overflow, zero divide, etc., can cause abnormal termination. In that case GRAPHE is not called, and the plot tape will not have the proper "end-of-tape" record.

6. SAMPLE INPUT/OUTPUT

6.1 Input Data Form

<u>PLOT IDENTIFICATION</u>	
<u>Title for Diagram:</u>	
* 1 _____ 72	
<u>Labels for Axes</u> (cc 1-36 for x-axis; cc 37-72 for y-axis):	
* 1 _____ 36 37 _____ 72	

<u>SCALING DATA</u>	
<u>Item:</u>	<u>Entry:</u>
Length of X-axis, inches	* _____
Minimum value for X-axis	_____
Maximum value for X-axis	_____
Length of Y-axis, inches	_____
Minimum value for Y-axis	_____
Maximum value for Y-axis	_____

<u>DEBUG OPTION</u>	
Enter 0 for no debug printout:	* _____

<u>CONTOURS REQUESTED</u>	
<u>Function code:</u> 1 = Pressure; 2 = Density; 3 = Enthalpy -1 = "return to Main Program"	* _____
<u>Number of contours</u> for this function (100 max.)	* _____
<u>Values of contours</u> requested:	
_____	_____
_____	_____
_____	_____
_____	_____

* Start a new card

6.2 Sample Problem Input Data

```

1 THERMODYNAMIC PROPERTIES OF FLUORINOL
2 FLUORINOL 100
3
1 180 700 20.0
4
1 9 .99 1 5 14.696 50 100 300 700 700.1
5
2 2 1. 1.E-10
6
2
CF3CH2OH      100.0 11.8 -3742.6 -25.97
WATER         18.016 12.144 -4203.9 -26.75
9
2
5.391      .074913 -.00005309 1.3501E-8
7.136      .00264 4.50E-8 0.
10
C
499.83 48.652 8755.63 344 1.3736 295.15
647.3 218.2 9717. 373.15 1. 277.15
99
T-S DIAGRAM FLUORINOL 100 7207310800
ENTROPY (BTU/LB-F) TEMPERATURE (F)
16 .08 .72 12 150 750
0
1
7 1 5 14.696 50 100 300 700
2
3 .5 2 8
3
16 80 100 120 140 160 180 200 220 240 260 280 300 320 340
360 380
-1

```


6.3 Sample Problem Printout

```

T-S DIAGRAM      FLUX/INFL 100      7207310800
PROPERTY (ATU/LG-F)
0.100E 02 0.4000E-01 0.7200E 00 0.1200E 02 0.1500E 03 0.7500E 03
27 9

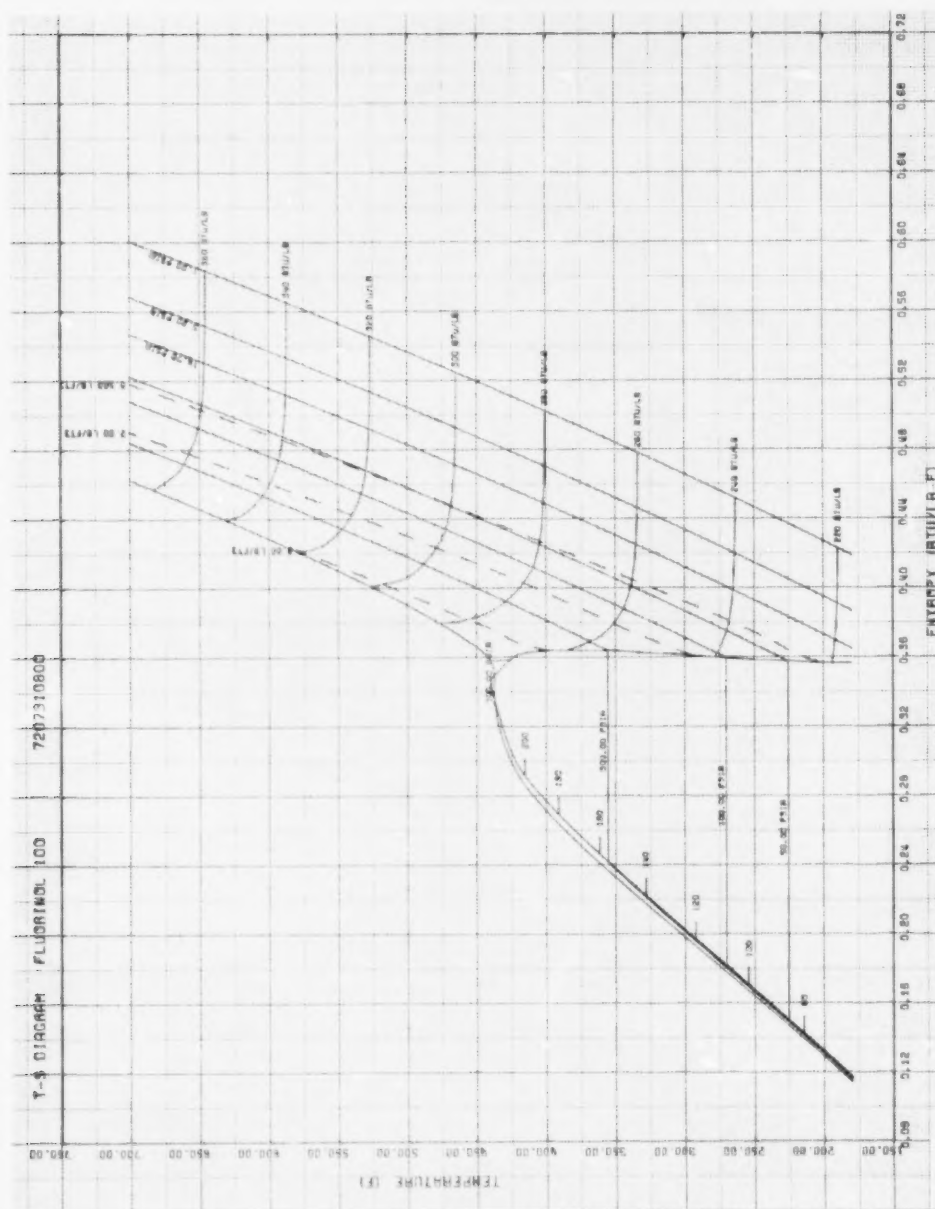
CONTOURS PLOTTED FOR FUNCTION 1
0.1000E 01 0.5000E 01 0.1000E 02 0.5000E 02 0.1000E 03 0.3000E 03 0.7000E 03

CONTOURS PLOTTED FOR FUNCTION 2
0.4000E 00 0.2000E 01 0.2000E 01

CONTOURS PLOTTED FOR FUNCTION 3
0.2200E 03 0.2400E 03 0.2600E 03 0.2800E 03 0.3000E 03 0.3200E 03 0.3400E 03 0.3600E 03

```

6.4 Sample Problem Diagram



7. COMPUTER PROGRAMS

PAGE 1

C	PROGRAM F1393	10
C		20
C		30
C	SEE SUBROUTINE "TSPLT" FOR DEFINITION OF NAMES USED IN PLOT ROUTI	40
C		50
C		60
C		70
C		80
C	DECLARATIVE SECTION	90
C	COMMON DB(1600), GA(20,20,3), GK(20,20,3)	100
C	COMMON/LITD/ NAME(3,20)	110
C		120
C	FILE SECTION	130
C	900 FORMAT(G1.0)	140
C	901 FORMAT(3A4, (G1.0))	150
C		160
C	INPUT SECTION	170
C		180
	LNMX = 13 INITIALIZE CONTR INE + PROG NO.	190
	CALL CDP(DB, LN, LNMX, KTE, KIN)	200
	CALL HEADER(-1393)	210
C	READ LIST NUMBER, CONTROL LISTS	220
	5 CALL CDP1	230
	GO TO (11, 5, 13, 14, 15, 16, 17, 18, 19, 20, 5, 5, 23), LN	240
	IF (LN.EQ. 99) GO TO 30	250
	CALL GRAPHE	260
	CALL EXIT	270
C	INITIALIZE PROBLEM-SET	280
	11 CALL ZERO(IN, 1, 4000)	290
C	SET DEFAULT OPTIONS	300
	DB(7) = .1	310
	DB(8) = 2000.	320
	DB(9) = -300.	330
	DB(10) = 1000.	340
	DB(32) = 1.0	350
	DB(36) = 150.	360
	DB(37) = 1E-5	370
	GO TO 5	380
C	READ PROBLEM-DATA LISTS	390
C	LIST 3, TEMPERATURE GRID	400
	13 READ (5,900) (DB(I), I=2,6)	410
	GO TO 5	420
C	LIST 4, PRESSURE GRID	430
	14 READ (5,900) DB(12), N, (DB(I + 50), I = 1, N)	440
	DB(13) = N	450
	GO TO 5	460
C	LIST 5, SYSTEM COMPOSITION	470
	15 READ (5,900) DB(19), N, (DB(I+100), I=1,N)	480
	DB(20) = N	490
	GO TO 5	500
C	LIST 6, MOLECULAR WEIGHTS AND ANTOINE	510
C	CONSTANTS	520
	16 READ (5,900) N	530
	DB(21) = N	540
	DO 160 I = 1,N	550

160 READ (5,901)	(NAME(J,1), J=1,3), DB(I+120), DB(I+140),	560
1	DB(I+160), DB(I+180)	570
GO TO 5		580
C	LIST 7, LIQ. ACT. COEF. DATA FOR A(I,J)	590
17 READ (5,900)	N, DB(23), (I, J, (GA(I,J,K), K=1,3),	600
1	(GA(J,I,K), K=1,3), I1=1,N)	610
DB(22) = N		620
GO TO 5		630
C	LIST 8, LIQ. ACT. COEF. DATA FOR C(I,J)	640
18 READ (5,900)	N, DB(25), (I, J, (GK(MIND(I,J), MAX0(I,J), K),	650
1	K=1,3), I1=1,N)	660
DB(24) = N		670
GO TO 5		680
C	LIST 9, IDEAL GAS HEAT CAPACITY CONSTANTS	690
19 READ (5,900)	N, ((DB(I + J*20 + 180), J=1,4), I=1,N)	700
DB(26) = N		710
GO TO 5		720
C	LIST 10, CRITICAL PROPERTIES, HEAT OF	730
C	VAPORIZATION, LIQUID DENSITY	740
20 READ (5,900)	N, ((DB(I + 20*J + 300), J=1,6), I = 1,N)	750
DB(27) = N		760
GO TO 5		770
C	LIST 13, CONTROL DATA	780
23 READ (5,900)	(DB(I), I = 31,37)	790
GO TO 5		800
C	CHECK AND PRINT INPUT DATA	810
C		820
30 CALL CHECK(INF)		830
IF (NE .GT. 0) GO TO 5		840
C		850
C	COMPUTATION SECTION	860
C	INITIALIZE TRIAL-ERROR CONTROLS	870
40 CALL CDP2		880
C	SOLVE MODEL	890
50	KEE = 0	900
CALL MODEL(KEE)		910
IF (KEE .GT. 0) GO TO 60		920
C	CHECK TRIAL-ERROR CALCULATIONS	930
CALL CDP3		940
IF (KTE .GT. 0) GO TO 50		950
C		960
C	OUTPUT SECTION	970
C	PRINT CASE RESULTS	980
60 CALL OUTPUT(KEE)		990
C	PRINT T-E SUMMARY, STORE CASE SUMMARY	1000
C	AND INCREMENT CASE	1010
CALL CDP4		1020
IF (KIN .FO. 1) GO TO 40		1030
CALL TSPLOT		1040
GO TO 5		1050
END		1060

	SUBROUTINE ADJBND(X,Y,N,LL)	10
C		20
C		30
C	PURPOSE	40
C		50
C	SOURCE ENTROPIES FOR THE LIQUID SIDE OF THE SATURATION CURVE.	60
C	ARRAY RE. ARE MADE TO AGREE WITH VALUES USED TO PLOT THAT	70
C	CURVE. ARRAY BXY. CHANGES ARE MADE ONLY IF MONOTL DELETED ANY	80
C	POINTS.	90
C		100
C	X,Y ARE ARRAYS OF N DENSE POINTS USED TO PLOT THE	110
C	SATURATION CURVE (BOUNDARY).	120
C	LL IS THE INDEX TO THE LARGEST TEMPERATURE VALUE IN	130
C	THE SOURCE DATA FOR THE BOUNDARY.	140
C		150
C		160
C	SUBROUTINES CALLED	170
C	FINDXC	180
C		190
C	COMMON DB(800),TG(50),PG(50),RE(50,8)	200
C		210
C	DIMENSION X(1),Y(1)	220
C		230
	DO 40 I = 1,LL	240
	YT = TG(I)	250
	XT = RE(I,4)	260
	CALL FINDXC(X,Y,N,YT,XT)	270
40	RE(I,4) = XT	280
	RETURN	290
	END	300

	SUBROUTINE RMDRY(N,L2,K,X,Y)	10
C		20
C		30
C	PURPOSE	40
C		50
C	COORDINATES FOR THE SATURATION CURVE ARE COPIED FROM SOURCE DAT	60
C	AND PLACED IN CLOCKWISE ORDER IN X,Y. ON RETURN, L2 IS THE	70
C	INDEX TO MAXIMUM Y-VALUE IN THE SOURCE DATA. N IS THE SIZE OF	80
C	THE SOURCE ARRAYS.	90
C		100
C	COMMON DB(800),TG(50),PG(50),RE(50,8),Z1301(2700),RG(50,50,3)	110
C		120
C	DIMENSION X(1),Y(1)	130
C		140
	L2 = 0	150
	DO 10 I = 1,N	160
	IF (RE(I,1) .EQ. 0.) GO TO 20	170
	L2 = I	180
10	CONTINUE	190
20	L = 2*L2	200
	DO 40 I = 1,L2	210
	J = L+3-I	220
	X(I) = RE(I,4)	230
	X(J) = RE(I,8)	240
	IF (K .NE. 0) GO TO 30	250
	Y(I) = TG(I)	260
	Y(J) = TG(I)	270
	GO TO 40	280
30	Y(I) = RE(I,K)	290
	Y(J) = RE(I,K+4)	300
40	CONTINUE	310
	X(L2+1) = X(L2)	320
	X(L2+2) = X(L2+3)	330
	Y(L2+1) = Y(L2)	340
	Y(L2+2) = Y(L2+3)	350
	L2 = L2+1	360
	RETURN	370
	END	380
		390

	SUBROUTINE ROUNDZ(N,L2,K,Y,Z)	10
C		20
C		30
C	PURPOSE	40
C		50
C	Y-COORDINATES AND FUNCTION VALUES ALONG THE SATURATION CURVE	60
C	ARE COPIED FROM THE SOURCE DATA AND PUT IN CLOCKWISE ORDER IN	70
C	ARRAYS Y,Z. ON RETURN, L2 IS THE INDEX TO MAXIMUM Y-VALUE IN	80
C	THE SOURCE DATA. N IS THE SIZE OF THE SOURCE ARRAYS.	90
C		100
C	COMMON DB(800),TG(50),PG(50),RE(50,8)	110
C		120
C	DIMENSION Y(1),Z(1)	130
C		140
	L2 = 0	150
	DO 10 I = 1,N	160
	IF (RE(I,1) .EQ. 0.) GO TO 20	170
	L2 = I	180
10	CONTINUE	190
20	L = 2*L2+2	200
	DO 30 I = 1,L2	210
	J = L+1-I	220
	Y(I) = TG(I)	230
	Y(J) = TG(I)	240
	Z(I) = RE(I,K)	250
30	Z(J) = RE(I,K+4)	260
	Y(L2+1) = Y(L2)	270
	Y(L2+2) = Y(L2+3)	280
	Z(L2+1) = Z(L2)	290
	Z(L2+2) = Z(L2+3)	300
	RETURN	310
	END	320
		330

C	SUBROUTINE CONRD(X,Y,N,C,XC,XX,YY)	10
C		20
C	PURPOSE	30
C		40
C	THE N VALUES OF ARRAY Y ARE SEARCHED TO FIND IF THE VALUE, C,	50
C	IS INCLUDED. IF IT IS, A CORRESPONDING VALUE, XC, IS FOUND FROM	60
C	ARRAY X BY INTERPOLATION. IF C WAS NOT FOUND IN Y, THEN XC IS	70
C	SET TO A FLAG VALUE (-1.E70 OR -2.E60).	80
C		90
C	XX,YY ARE INCLUDED TO PASS THE LOCATION OF THESE ARRAYS TO	100
C	SUBROUTINE FINDXC.	110
C		120
C	SUBROUTINES CALLED	130
C	DENSFY, FINDXC	140
C		150
C	DIMENSION X(1),Y(1),XX(1),YY(1)	160
C		170
	XC = -1.E70	180
	IF (N .LT. 2) GO TO 30	190
	EPS = ABS(C*C)*1.E-4	200
	IF ((C-Y(1))*(C-Y(N)) .GT. EPS) GO TO 30	210
	CALL DENSFY(X,Y,N,NPT,XX,YY)	220
	CALL FINDXC(XX,YY,NPT,C,XC)	230
	IF (XC .LT. -1.E60) XC=-2.E60	240
30	RETURN	250
	END	260
		270
		280

	SUBROUTINE DENSFY(X,Y,N,NP,XX,YY)	10
C		20
C		30
C	PURPOSE	40
C		50
C	DENSFY SETS UP A CALL TO FLINE TO OBTAIN A DENSE SET OF NP POIN	60
C	IN XX,YY USING THE N PAIRS IN X,Y. IF N IS NOT GREATER THAN	70
C	2, THE CALL TO FLINE IS NOT MADE.	80
C		90
C		100
C	SUBROUTINES CALLED	110
C	FLINE	120
C		130
C	COMMON /FLIP/ ISKIP,IK,NEAR	140
C		150
C	DIMENSION X(1),Y(1),XX(1),YY(1)	160
		170
	IF (N .GT. 2) GO TO 10	180
	XX(1) = X(1)	190
	YY(1) = Y(1)	200
	XX(2) = X(2)	210
	YY(2) = Y(2)	220
	NP = 2	230
	GO TO 20	240
10	ISKSV = ISKIP	250
	NRSV = NEAR	260
	ISKIP = 0	270
	NEAR = 0	280
	IK = 0	290
	CALL FLINE(X,Y,-N,1,0,0,XX,YY)	300
	NP = IK	310
	ISKIP = ISKSV	320
	NEAR = NRSV	330
20	RETURN	340
	END	350

	SUBROUTINE ENTHAL(X,Y,ICT,XB,YB,NX,XX,YY)	10
		20
C		30
C	PURPOSE	40
C		50
C	X,Y ARE ARRAYS WITH ICT PAIRS OF COORDINATES FOR THE CURRENT	60
C	ISENTHALP. XB,YB ARE THE NX PAIRS OF COORDINATES FOR ANY	70
C	INTERSECTIONS OF THE ISENTHALP WITH THE SATURATION CURVE.	80
C	XX,YY ARE USED TO PASS THE LOCATION OF THESE ARRAYS TO FLINE.	90
C		100
C	ENTHAL PLOTS THE ISENTHALP WHENEVER NX IS NOT 0.	110
C		120
C		130
C	SUBROUTINES CALLED	140
C	SCALXY, FLINE	150
C		160
	COMMON /CUT/ XL,YL,XR,YR,YLIT	170
	COMMON /FLIP/ ISKIP,IK,NEAR	180
C		190
	DIMENSION X(1),Y(1),XB(1),YB(1),XX(1),YY(1)	200
C		210
	NB = 0	220
	DO 10 I = 1,ICT	230
	IF (Y(I) .LE. YB(NX)) NB=I	240
10	CONTINUE	250
	IF (NB .LT. 3) GO TO 15	260
	IK = 0	270
	ISKIP = 1	280
	X1S = X(NB+1)	290
	Y1S = Y(NB+1)	300
	X2S = X(NB+2)	310
	Y2S = Y(NB+2)	320
	CALL SCALXY(X,Y,NB)	330
	CALL FLINE(X,Y,-NB+1,NB-1,2,XX,YY)	340
	X(NB+1) = X1S	350
	Y(NB+1) = Y1S	360
	X(NB+2) = X2S	370
	Y(NB+2) = Y2S	380
		390
15	IF (NX .EQ. 1) GO TO 100	400
	NT = 0	410
	DO 20 I = 1,ICT	420
	IF (Y(I) .GE. YB(1)) NT=NT+1	430
20	CONTINUE	440
	IF (NT .LT. 7) GO TO 200	450
	N1 = ICT+1-NT	460
	IK = 0	470
	CALL SCALXY(X(N1),Y(N1),NT)	480
	CALL FLINE(X(N1),Y(N1),-NT+1,NT-1,2,XX,YY)	490
	GO TO 200	500
100	IF ((ICT-NB) .LT. 2) GO TO 200	510
	IK = 0	520
	ISKIP = 0	530
	CALL FLINE(X,Y,-ICT+1,0,0,XX,YY)	540
	ISKIP = 1	550
	NPTS = IK	

	IK	= 0	560
	IF (ABS(XR-XL)	.LT. 1.E-5) GO TO 200	570
	SL	= (YR-YL)/(XR-XL)	580
	DO 110 I	= 1,NPTS	590
	II	= I	600
	YC	= (XX(I)-XL)*SL+YL	610
	IF (YY(I)	.GE. YC) GO TO 120	620
110	CONTINUE		630
120	IF (II	.GE. NPTS) GO TO 200	640
	DO 130 I	= 1,ICT	650
	N1	= I	660
	IF (Y(I)	.GE. YY(II)) GO TO 140	670
130	CONTINUE		680
140	N1	= N1-1	690
	Y(N1)	= YY(II)	700
	X(N1)	= XX(II)	710
	NH	= ICT+1-N1	720
	CALL SCALXY(X(N1),Y(N1),NH)		730
	CALL FLINF(X(N1),Y(N1),-NH,1,NH-1,2,XX,YY)		740
200	RETURN		750
	END		760

	SUBROUTINE FINDXC(X,Y,N,C,XC)	10
C		20
C		30
C	PURPOSE	40
C		50
C	X,Y ARE N PAIRS OF DENSE DATA. C IS THE CURRENT CONTOUR LEVEL.	60
C	ARRAY Y IS SEARCHED TO FIND IF IT CONTAINS C. IF NOT, A RETURN	70
C	MADE WITHOUT CHANGING XC. IF C WAS FOUND IN Y, THEN ON RETURN,	80
C	XC WILL BE THE CORRESPONDING VALUE OBTAINED FROM X BY INTERPOL-	90
C	ATION.	100
C		110
C		120
C	DIMENSION X(1),Y(1)	130
C		140
	L = 1	150
10	L = L+1	160
	IF (L .GT. N) GO TO 30	170
	D1 = C-Y(L-1)	180
	D2 = C-Y(L)	190
	EC = AMAX1(ABS(D1),ABS(D2))	200
	EPS = EC*EC*.1E-5	210
	IF (D1*D2 .GT. EPS) GO TO 10	220
	IF (Y(L) .NE. Y(L-1)) GO TO 20	230
	XC = (X(L)+X(L-1))/2.	240
	GO TO 30	250
20	DD = ABS(D1/(Y(L)-Y(L-1)))	260
	XC = DD*(X(L)-X(L-1))+X(L-1)	270
30	RETURN	280
	END	290

	SUBROUTINE FUN1(IP,IY,NP,N,U,V)	10
C		20
C		30
C	PURPOSE	40
C		50
C	FUN1 SCANS THE SINGLE PHASE DATA AT ALL NP PRESSURES AT THE	60
C	Y-VALUE INDICATED BY IY. IP IS USED TO CONTROL WHETHER THE SCA	70
C	IS MADE FOR THE LIQUID SIDE (IP=1) OR THE GAS SIDE (IP=2).	80
C		90
C	ON RETURN ARRAYS U,V CONTAIN THE N PAIRS OF ENTROPY, PRESSURE	100
C	DATA.	110
C		120
C	COMMON DP(R00),TG(50),PG(50),RE(50,8),Z1301(2700),RG(50,50,3)	130
C		140
C	DIMENSION U(1),V(1)	150
C		160
	IF (IP .EQ. 2) GO TO 20	170
	N = 0	180
	BPL = 1.E70	190
	IF (RE(IY,1) .NE. 0.) BPL=RE(IY,4)	200
	DO 10 J1 = 1,NP	210
	J = NP+1-J1	220
	IF (RG(IY,J,1) .NE. 0.) GO TO 5	230
	IF (RG(IY,J,2) .EQ. 0. .AND. RG(IY,J,3) .EQ. 0.) GO TO 10	240
5	CONTINUE	250
	X = RG(IY,J,3)	260
	IF (X .GE. BPL) GO TO 10	270
	N = N+1	280
	U(N) = X	290
	V(N) = PG(J)	300
10	CONTINUE	310
	IF (RPL .GT. 1.E60) GO TO 50	320
	N = N+1	330
	U(N) = BPL	340
	V(N) = RE(IY,1)	350
	GO TO 50	360
20	N = 0	370
	BPR = -1.E70	380
	IF (RE(IY,5) .EQ. 0.) GO TO 30	390
	BPR = RE(IY,8)	400
	N = 1	410
	U(1) = BPR	420
	V(1) = RE(IY,5)	430
30	DO 40 J1 = 1,NP	440
	J = NP+1-J1	450
	IF (RG(IY,J,1) .NE. 0.) GO TO 35	460
	IF (RG(IY,J,2) .EQ. 0. .AND. RG(IY,J,3) .EQ. 0.) GO TO 40	470
35	CONTINUE	480
	X = RG(IY,J,3)	490
	IF (X .LE. BPR) GO TO 40	500
	N = N+1	510
	U(N) = X	520
	V(N) = PG(J)	530
40	CONTINUE	540
		550

50 RETURN
END

560
570

	SUBROUTINE FUN23(IY,IMK,NP,N,U,V,IER)	10
C		20
C		30
C	PURPOSE	40
C		50
C	IMK IS A FLAG IDENTIFYING THE CONTOUR FUNCTION CURRENTLY SOUGHT	60
C	IMK=1 FOR DENSITY; IMK=2 FOR ENTHALPY.	70
C		80
C	SINGLE PHASE DATA IS SCANNED AT ALL NP PRESSURES AT THE Y-VALUE	90
C	INDEXED BY IY. ON RETURN, ARRAYS U,V CONTAIN THE N PAIRS OF	100
C	ENTROPY,FUNCTION DATA.	110
C		120
C	IER IS THE ERROR CODE WHICH IS SET TO 3 IF IMK IS NOT EITHER 1	130
C		140
C		150
C	COMMON DB(800),TG(50),PG(50),RE(50,8),Z1301(2700),RG(50,50,3)	160
C		170
C	DIMENSION U(1),V(1)	180
C		190
	IER = 0	200
	IF (IMK .EQ. 1 .OR. IMK .EQ. 2) GO TO 10	210
	IER = 3	220
10	GO TO 40	230
	N = 0	240
	BPR = -1.E70	250
	IF (RE(IY,5) .EQ. 0.) GO TO 20	260
	BPR = RE(IY,8)	270
	N = 1	280
	U(1) = BPR	290
	V(1) = RE(IY,IMK+5)	300
20	DO 30 J1 = 1,NP	310
	J = NP+1-J1	320
	IF (RG(IY,J,1) .NE. 0.) GO TO 25	330
	IF (RG(IY,J,2) .EQ. 0. .AND. RG(IY,J,3) .EQ. 0.) GO TO 30	340
25	CONTINUE	350
	X = RG(IY,J,3)	360
	IF (X .LE. 0.) GO TO 30	370
	N = N+1	380
	U(N) = X	390
	V(N) = RG(IY,J,IMK)	400
30	CONTINUE	410
40	RETURN	420
	END	430

	SUBROUTINE IYBIG(Y,N,IB)	10
C		20
C		30
C	PURPOSE	40
C		50
C	ON RETURN, IB IS THE INDEX TO THE MAXIMUM VALUE IN ARRAY Y.	60
C	N IS THE NUMBER OF DATA VALUES IN ARRAY Y.	70
C		80
C		90
	DIMENSION Y(1)	100
C		110
	H = Y(1)	120
	IB = 1	130
	DO 10 I = 2,N	140
	IF (Y(I) .LE. H) GO TO 10	150
	H = Y(I)	160
	IB = I	170
10	CONTINUE	180
	RETURN	190
	END	200

C	SUBROUTINE KOK(IMK,L2,C,IC)	10
C		20
C		30
C	PURPOSE	40
C		50
C	IMK IS A CODE TO IDENTIFY THE FUNCTION. 0=PRESSURE;	60
C	1= DENSITY; 2= ENTHALPY. L2 IS THE INDEX TO THE MAXIMUM	70
C	TEMPERATURE AT WHICH DATA IS GIVEN FOR THE SATURATION CURVE.	80
C	C IS THE CURRENT VALUE FOR A CONTOUR.	90
C		100
C	ON RETURN, IC=0 IF THE VALUE FOR C IS REJECTED; IF C IS ACCEPT	110
C	IC=1, ALL PRESSURE CONTOURS (IMK=0) ARE ACCEPTED. DENSITY	120
C	CONTOURS ARE REJECTED FOR C GREATER THAN THE DENSITY AT L2 ON	130
C	THE GAS SIDE OF THE SATURATION DATA. ENTHALPY CONTOURS ARE	140
C	REJECTED IF C IS LESS THAN THE ENTHALPY AT THE LOWEST TEMPERATU	150
C	ON THE GAS SIDE OF THE SATURATION DATA.	160
C		170
C		180
C	COMMON DR(800),TG(50),PG(50),RE(50,8),Z1301(2700),RG(50,50,3)	190
C		200
	J = IMK+1	210
	IC = 1	220
	GO TO (30,10,20),J	230
10	IF (C .GT. RE(L2,6)) IC=0	240
	GO TO 30	250
20	IF (C .LT. RE(1,7)) IC=0	260
30	RETURN	270
	END	280

	SUBROUTINE MARK(X,Y,N,XB,YB,NX,IMK,C)	10
C		20
C		30
C	PURPOSE	40
C		50
C	MARK PLACES LABELS ON THE PLOTTED CONTOURS.	60
C		70
C	X,Y ARE N PAIRS OF DENSE COORDINATES FOR THE PLOT. XB,YB ARE	80
C	NX PAIRS OF COORDINATES FOR ANY INTERSECTIONS OF THE CONTOUR	90
C	C WITH THE SATURATION CURVE. IMK IDENTIFIES THE CONTOUR FUNCTI	100
C	BEING PLOTTED.	110
C		120
C		130
C	SUBROUTINES CALLED	140
C	NUMBER, SYMBOL	150
C		160
C	COMMON /SKAL/ XLEN,XMIN,XDEL,YLEN,YMIN,YDEL	170
C		180
C	DIMENSION X(1),Y(1),XB(1),YB(1),UNITS(6)	190
C		200
C	DATA UNITS/' PSI','A ',' LB/','FT3 ',' BTU','/LB '	210
C		220
	ALF = 0.	230
	RTOD = 180./3.1415927	240
	K = IMK+1	250
	NDIG = -1	260
	GO TO (10,20,30),K	270
10	NDIG = 2	280
	IF (NX .EQ. 2) GO TO 15	290
	IF (NX .EQ. 0) GO TO 12	300
	XP = (X(1)-XMIN)/XDEL-.25	310
	YP = (Y(1)-YMIN)/YDEL-.04	320
	GO TO 40	330
12	X0 = (X(N)-X(N-5))/XDEL	340
	Y0 = (Y(N)-Y(N-5))/YDEL	350
	ALF = ATAN2(Y0,X0)	360
	XD = COS(ALF)*.04	370
	YD = SIN(ALF)*.04	380
	ALF = ALF*RTOD	390
	XP = (X(N)-XMIN)/XDEL-XD	400
	YP = (Y(N)-YMIN)/YDEL-YD	410
	GO TO 40	420
15	XP = (XB(2)-XB(1))/XDEL	430
	YP = (YB(2)-YB(1))/YDEL	440
	ALF = ATAN2(YP,XP)*RTOD	450
	XP = ((XB(2)+XB(1))/2.-XMIN)/XDEL-.2	460
	YP = ((YB(2)+YB(1))/2.-YMIN)/YDEL+.04	470
	GO TO 40	480
20	ALF = 90.	490
	XP = (X(N)-XMIN)/XDEL+.04	500
	YP = (Y(N)-YMIN)/YDEL+.08	510
	CF = ABS(C)	520
	IEX = 0	530
32	IF (CF .GE. 1.) GO TO 34	540
	CF = 10.*CF	550

	IEX	= IEX+1	560
	GO TO 32		570
34	NDIG	= IEX+2	580
	NDIG	= MIN0(NDIG,6)	590
	GO TO 40		600
30	XP	= (X(1)-XMIN)/XDEL+.08	610
	YP	= (Y(1)-YMIN)/YDEL-.04	620
40	CALL NUMBER(XP,YP,.08,C,ALF,NDIG)		630
	KU	= 2*IMK+1	640
	CALL SYMBOL(999.,999.,.08,UNITS(KU),ALF,8)		650
	RETURN		660
	END		670

C	SUBROUTINE MONOTL(X,Y,N,L,IER)	10
C		20
C	PURPOSE	30
C		40
C	MONOTL CHECKS THE LIQUID SIDE OF THE BOUNDARY DATA FOR THE	50
C	SATURATION CURVE. A PAIR OF COORDINATES IS DELETED FOR ANY	60
C	X(I) FOR WHICH X(I) IS LESS THAN X(I-1).	70
C		80
C	ON RETURN, L CONTAINS THE NUMBER OF PAIRS X,Y REMAINING. IER	90
C	IS THE ERROR CODE WHICH IS SET TO 1 IF LESS THAN THREE POINTS	100
C	REMAIN IN X,Y.	110
C		120
C		130
C		140
C	DIMENSION X(1),Y(1)	150
C		160
	IER = 0	170
	NM1 = N-1	180
	I = 1	190
10	I = I+1	200
	IF (I .GT. L) GO TO 30	210
	IF (X(I) .GE. X(I-1)) GO TO 10	220
	DO 20 K = I,NM1	230
	X(K) = X(K+1)	240
20	Y(K) = Y(K+1)	250
	N = N-1	260
	NM1 = N-1	270
	L = L-1	280
	I = I-1	290
	IF (N .GT. 2) GO TO 10	300
	IER = 1	310
30	RETURN	320
	END	330

	SUBROUTINE SCALD(X,Y,N)	10
C		20
C		30
C	PURPOSE	40
C		50
C	X,Y ARE N PAIRS OF DATA. ON RETURN, Y(N+1) CONTAINS THE MINIMU	60
C	Y-VALUE: Y(N+2) CONTAINS (YMAX-YMIN)/YLEN.	70
C		80
C		90
C	COMMON /SKAL/ XLEN,XMIN,XDEL,YLEN,YMIN,YDEL	100
C		110
C	DIMENSION X(1),Y(1)	120
		130
	S = Y(1)	140
	B = S	150
	DO 10 I = 2,N	160
	IF (Y(I) .GT. B) B=Y(I)	170
	IF (Y(I) .LT. S) S=Y(I)	180
10	CONTINUE	190
	Y(N+1) = S	200
	Y(N+2) = (B-S)/YLEN	210
	RETURN	220
	END	230

	SUBROUTINE SCALUV(U,V,N)	10
C		20
C		30
C	PURPOSE	40
C		50
C	U,V ARE N PAIRS OF DATA. A CALL IS FIRST MADE TO SCALD. ON	60
C	RETURN FROM SCALUV, V(N+1) AND V(N+2) WILL BE AS DETERMINED	70
C	IN SCALD. U(N+1) WILL CONTAIN THE MINIMUM U-VALUE. U(N+2)	80
C	WILL CONTAIN (UMAX-UMIN)/XLEN.	90
C		100
C		110
C	SUBROUTINES CALLED	120
C	SCALD	130
C		140
C	COMMON /SKAL/ XLEN,XMIN,XDEL,YLEN,YMIN,YDEL	150
C		160
C	DIMENSION U(1),V(1)	170
C		180
C	CALL SCALD(U,V,N)	190
	S = U(1)	200
	B = S	210
	DO 10 I = 1,N	220
	IF (U(I) .GT. B) B=U(I)	230
	IF (U(I) .LT. S) S=U(I)	240
10	CONTINUE	250
	U(N+1) = S	260
	U(N+2) = (B-S)/XLEN	270
	RETURN	280
	END	290

	SUBROUTINE SCALXY(X,Y,N)	10
C		20
C		30
C	PURPOSE	40
C		50
C	X,Y ARE N PAIRS OF DATA. ON RETURN, X(N+1)=XMIN, X(N+2)=XDEL,	60
C	Y(N+1)=YMIN, Y(N+2)=YDEL.	70
C		80
C		90
C	COMMON /SKAL/ XLEN,XMIN,XDEL,YLEN,YMIN,YDEL	100
C		110
C	DIMENSION X(1),Y(1)	120
		130
	X(N+1) = XMIN	140
	X(N+2) = XDEL	150
	Y(N+1) = YMIN	160
	Y(N+2) = YDEL	170
	RETURN	180
	END	190

	SUBROUTINE SERT(IMK,X,Y,N,XB,YB,NX,IER)	10
C		20
C		30
C	PURPOSE	40
C		50
C	SERT INSERTS POINTS OF INTERSECTION INTO THE X,Y COORDINATES	60
C	FOR A CONTOUR. XB,YB ARE THE NX PAIRS OF COORDINATES FOR	70
C	INTERSECTIONS.	80
C		90
C	IER IS THE ERROR CODE WHICH IS SET TO 4 IF THE FUNCTION CODE	100
C	(IMK) IS NOT EITHER 1 OR 2.	110
C		120
C		130
C	DIMENSION X(1),Y(1),XB(1),YB(1)	140
C		150
	IER = 0	160
	IF (NX .EQ. 0) GO TO 70	170
	IF (IMK .EQ. 1) GO TO 10	180
	IF (IMK .EQ. 2) GO TO 40	190
	IER = 4	200
	GO TO 70	210
10	XR = XB(1)	220
	YR = YB(1)	230
	IF (NX .EQ. 1) GO TO 20	240
	XR = XB(2)	250
	YR = YB(2)	260
20	DO 30 I1 = 1,N	270
	I = N+2-I1	280
	X(I) = X(I-1)	290
30	Y(I) = Y(I-1)	300
	N = N+1	310
	X(1) = XR	320
	Y(1) = YR	330
	GO TO 70	340
40	DO 60 I = 1,NX	350
	U = XB(I)	360
	V = YB(I)	370
	J = 0	380
45	J = J+1	390
	IF (J .GT. N) GO TO 55	400
	IF (V .GT. Y(J)) GO TO 45	410
	DO 50 K1 = J,N	420
	K = N+1-K1+J	430
	X(K) = X(K-1)	440
50	Y(K) = Y(K-1)	450
55	X(J) = U	460
	Y(J) = V	470
	N = N+1	480
60	CONTINUE	490
70	RETURN	500
	END	510

SUBROUTINE TICS(BXY,BY,BYZ,BZ,C,NBZ,NBY)

PURPOSE

TICS PLOTS A 1/2" HORIZONTAL LINE INSIDE THE SATURATION CURVE BOUNDARY WHERE AN ISENTHALP INTERSECTS THE LIQUID SIDE OF THE BOUNDARY. THE LINE IS LABELED WITH THE VALUE OF C.

ARRAYS BXY,BY ARE NBY PAIRS OF DENSE COORDINATES OF THE BOUNDARY BYZ,BZ ARE NBZ PAIRS OF DENSE DATA FOR TEMPERATURE AND FUNCTION VALUE ALONG THE BOUNDARY.

SUBROUTINES CALLED

FINDXC, GRAPH, NUMBER

COMMON /SKAL/ XLEN,XMIN,XDEL,YLEN,YMIN,YDEL

DIMENSION PXY(1),BY(1),BYZ(1),BZ(1),X(4),Y(4)

YC = -1.E70
CALL FINDXC(BYZ,BZ,NBZ,C,YC)
IF (YC .LT. -1.E60) RETURN
CALL FINDXC(PXY,BY,NBY,YC,XC)

X(1) = XC
Y(1) = YC
Y(2) = YC
X(2) = XC+XDEL/2.

CALL GRAPH(2,X,Y,0)
XP = (XC-XMIN)/XDEL+.54
YP = (YC-YMIN)/YDEL+.04
CALL NUMBER(XP,YP,.08,C,0,-1)
RETURN
END

C	SUBROUTINE TCOLOT	10
C		20
C		30
C	SUBROUTINES CALLED	40
C	ADJEND, ENDRY, BOUND7, COORD, DENSFY, ENTHAL, FLINE, FUN1,	50
C	FUN23, GRAP, GRAPHE, GRAPHI, IYBIG, KOK, MARK, MONOTL,	60
C	SCALO, SCALOV, SCALXY, SEPT, TICS, XTENT, YSECT	70
C		80
C	DEFINITIONS	90
C		100
C	AXISID ARRAY OF 72 CHARACTERS FOR AXES LABELS (I	110
C	BXY ARRAY(1500) OF X-COORD. FOR BOUNDARY	120
C	BY ARRAY(1500) OF Y-COORD. FOR BOUNDARY (USED WITH BXY)	130
C	BYZ ARRAY(1500) OF Y-COORD. FOR FUNCTION ON BOUNDARY	140
C	BZ ARRAY (1500) OF FUNCTION VALUES (USED WITH BYZ)	150
C	C CURRENT CONTOUR VALUE	160
C	IC FLAG FOR ACCEPTING "C" (0=REJECT; 1=ACCEPT)	170
C	IDRUG FLAG FOR DEBUG PRINTOUT (=0 FOR NO PRINTOUT) (I	180
C	IK COUNT OF POINTS RETURNED FROM FLINE	190
C	IMK SYMBOL KODE (= KONTUR-1)	200
C	ISKIP FLAG FOR PLOTTING IN FLINE (0=NO PLOT; 1= PLOT)	210
C	KONTUR I.D. FOR CONTOUR FUNCTION (1=P12=D13=H)	220
C	L2 NUMBER OF PAIRS OF POINTS IN SAT.DAT	230
C	LL INDEX TO HIGHEST DATA POINT ON SAT. CURVE DATA	240
C	NBY NUMBER OF DENSE POINTS IN ARRAYS BXY,BY	250
C	NBZ NUMBER OF DENSE POINTS IN ARRAYS BYZ,BZ	260
C	NEAR FLAG TO START PLOT AT NEAREST POINT (1= USE NEAR END	270
C	NL NUMBER OF CONTOURS REQUESTED (I	280
C	NP NUMBER OF GRID PRESSURES	290
C	NT NUMBER OF GRID TEMPERATURES	300
C	NX NUMBER OF POINTS WHERE "C" INTERSECTS SAT. CURVE	310
C	SCALES ARRAY(6) OF PLOT SCALING INFORMATION (SEE BELOW) (I	320
C	TITLE ARRAY OF 72 CHARACTERS FOR PLOT TITLE (I	330
C	XLEN LENGTH OF X-AXIS, INCHES (=SCALES(1))	340
C	XMIN MINIMUM X-VALUE FOR PLOT (=SCALES(2))	350
C	XMAX MAXIMUM X-VALUE FOR PLOT (=SCALES(3))	360
C	YLEN LENGTH OF Y-AXIS, INCHES (=SCALES(4))	370
C	YMIN MINIMUM Y-VALUE FOR PLOT (=SCALES(5))	380
C	YMAX MAXIMUM Y-VALUE FOR PLOT (=SCALES(6))	390
C	XDEL UNITS PER INCH ON X-AXIS	400
C	YDEL UNITS PER INCH ON Y-AXIS	410
C	XL X-VALUE AT HIGHEST SAT. DATA PAIR, LIQUID SIDE	420
C	XR X-VALUE AT HIGHEST SAT. DATA PAIR, GAS SIDE	430
C	YL Y-VALUE AT HIGHEST SAT. DATA PAIR, LIQUID SIDE	440
C	YR Y-VALUE AT HIGHEST SAT. DATA PAIR, GAS SIDE	450
C	YLIT SMALLER OF YL, YR	460
C	XX ARRAY(1500) OF DENSE DATA RETURNED FROM FLINE	470
C	YY ARRAY(1500) OF DENSE DATA RETURNED FROM FLINE	480
C	ZL ARRAY(NL) OF REQUESTED CONTOUR VALUES (I	490
C		500
C		510
C	ERROR CODES	520
C		530
C	1 FROM MONOTL LESS THAN 3 POINTS REMAIN ON BOUNDARY	540
C	2 NOT USED	550


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C      3 FROM FUN23      INVALID "IMK"      560
C      4 FROM SERT      INVALID "IMK"      570
C      ERROR MESSAGE      580
C      "FLINE - IK TOO BIG" MEANS THAT MORE THAN 1498 PTS WERE GENERA      590
C      600
C      610
C      620
C      SUBROUTINE TSPLOT      630
C      640
C      COMMON DB(400),TG(50),PG(50),RE(50,8),Z1301(2700),RG(50,50,3)      650
C      COMMON /FLIP/ ISKIP,IK,NEAR      660
C      COMMON /SKAL/ XLEN,XMIN,XDEL,YLEN,YMIN,YDEL      670
C      COMMON /CUT/ XL,YL,XR,YR,YLIT      680
C      690
C      DIMENSION TITLE(18),AXISID(18),SCALES(6),ZL(100),CPLT(100),      700
1      U(100),V(100),X(100),Y(100),XB(4),YB(4),IBIG(2),      710
2      BXY(1500),BY(1500),BYZ(1500),BZ(1500),XX(1500),YY(1500)      720
C      730
C      740
C      900 FORMAT(G1.0)      750
C      910 FORMAT(1PA4)      760
C      920 FORMAT(1H0,'ERROR ',I5/)      770
C      940 FORMAT(1X,10F12.4)      780
C      950 FORMAT(1H0,'BOUNDARY X,Y'//)      790
C      960 FORMAT(1H0,'BOUNDARY Z,Y'//)      800
C      970 FORMAT(1H0,'YSECT ',4E12.4/)      810
C      980 FORMAT(1H0,'CONTOURS PLOTTED FOR FUNCTION ',I3/(1X,10E12.4))      820
C      990 FORMAT(1H1,1PA4/1X,1BA4/1X,5E12.4/1X,2I5//)      830
C      840
C      NP = DB(13)      850
C      NT = AMIN1(2,*(DB(4)-DB(3))/DB(5),50.)      860
C      DO 30 I = 2,NT      870
C      TG(I-1) = TG(I)      880
C      DO 10 J = 1,8      890
10      RE(I-1,J) = RE(I,J)      900
C      DO 20 J = 1,50      910
C      DO 20 K = 1,3      920
20      RG(I-1,J,K) = RG(I,J,K)      930
30      CONTINUE      940
C      NT = NT-1      950
C      960
C      INPUT DESCRIPTIVE DATA FOR PLOT      970
C      980
C      READ(5,910) (TITLE(I),I=1,18)      990
C      READ(5,910) (AXISID(I),I=1,18)      1000
C      READ(5,900) (SCALES(I),I=1,6)      1010
C      READ(5,900) IDBUG      1020
C      WRITE(6,990) TITLE,AXISID,SCALES,NT,NP      1030
C      1040
C      INITIALIZE PLOT      1050
C      1060
C      CALL GRAPHI(0,-1,SCALES,1,TITLE,1,AXISID,0,0,0,0)      1070
C      1080
C      SAVE SCALING DATA AND PLOT BORDER      1090
C      1100

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	XLEN = SCALES(1)	1110
	XMIN = SCALES(2)	1120
	XMAX = SCALES(3)	1130
	XDFL = (XMAX-XMIN)/XLEN	1140
	YLEN = SCALES(4)	1150
	YMIN = SCALES(5)	1160
	YMAX = SCALES(6)	1170
	YDFL = (YMAX-YMIN)/YLEN	1180
	X(1) = XMIN	1190
	X(2) = XMAX	1200
	X(3) = XMAX	1210
	Y(1) = YMAX	1220
	Y(2) = YMAX	1230
	Y(3) = YMIN	1240
C		1250
C	FINISH BORDER PLOT	1260
C		1270
	CALL GRAPH(3,X,Y,0)	1280
	NEAR = 0	1290
	IER = 0	1300
C		1310
C	COLLECT AND ORDER BOUNDARY DATA	1320
C		1330
	CALL BNDRY(NT,L2,0,X,Y)	1340
	LL = L2-1	1350
	YBIG = TG(LL)	1360
	XL = X(LL)	1370
	YL = Y(LL)	1380
	XR = X(LL+3)	1390
	YR = Y(LL+3)	1400
	YLIT = AMIN1(YL,YR)	1410
C		1420
C	PLOT THE BOUNDARY AND SAVE COORD. (BXY,BY)	1430
C		1440
	NN = 2*L2	1450
	CALL MONOTL(X,Y,NN,L2,IER)	1460
	IF (IER.NE.0) GO TO 500	1470
	IF (IDBUG.EQ.0) GO TO 50	1480
	WRITE(6,950)	1490
	WRITE(6,940) (X(I),Y(I),I=1,NN)	1500
50	CONTINUE	1510
	CALL SCALXY(X,Y,NN)	1520
	ISKIP = 1	1530
	IK = 0	1540
	CALL FLINE(X,Y,-NN,1,0,0,BXY,RY)	1550
	IF (IDBUG.NE.0) WRITE(6,940) (BXY(I),BY(I),I=1,IK)	1560
	NBY = IK	1570
	CALL ADJBND(RXY,BY,NBY,LL)	1580
	IF (IDBUG.EQ.0) GO TO 70	1590
	DO 60 I = 1,NT	1600
60	WRITE(6,940) TG(I),(RE(I,J),J=1,8)	1610
70	CONTINUE	1620
	CALL IYBIG(RY,NBY,IBIG(1))	1630
C		1640
C	INPUT FUNCTION ID AND REQUESTED CONTOUR LEVELS	1650

C			1660
100	READ (5,900,END=510) KONTUR		1670
	IF (KONTUR .LT. 1) RETURN		1680
	IF (KONTUR .GT. 3) GO TO 510		1690
	IMK = KONTUR-1		1700
	IFLG = 0		1710
	READ (5,900,END=510) NL, (ZL(I), I=1,NL)		1720
C			1730
C	COLLECT AND ORDER FUNCTION DATA FOR BOUNDARY		1740
C			1750
	CALL BOUNDZ(NT,L2,IMK+1,Y,X)		1760
C			1770
C	DENSIFY AND SAVE BOUNDARY DATA. (BYZ,BZ)		1780
C			1790
	NN = 2*L2+2		1800
	IF (IDBUG .EQ. 0) GO TO 105		1810
	WRITE(6,960)		1820
	WRITE(6,940) (X(I),Y(I), I=1,NN)		1830
105	CONTINUE		1840
	CALL SCALUV(X,Y,NN)		1850
	Y(NN+1) = YMIN		1860
	Y(NN+2) = YDEL		1870
	CALL DENSFY(Y,X,NN,NBZ,BYZ,BZ)		1880
	IF (IDBUG .NE. 0) WRITE(6,940) (BYZ(I),BZ(I), I=1,NBZ)		1890
	CALL IYBIG(BYZ,NBZ,IBIG(2))		1900
C			1910
C	FIND POINTS FOR A CONTOUR AND PLOT		1920
C			1930
	NCPLT = 0		1940
	DO 210 KT = 1,NL		1950
	C = ZL(KT)		1960
	CALL KOK(IMK,L2,C,IC)		1970
	IF (IMK .EQ. 2 .AND. IC .EQ. 0) CALL TICS(BXY,BY,BYZ,BZ,C,		1980
	1 IBIG(2),IBIG(1))		1990
	IF (IC .EQ. 0) GO TO 210		2000
C			2010
C	LOCATE ANY BOUNDARY INTERSECTIONS		2020
C			2030
110	CALL YSECT(IYIG,BXY,BY,NBY,BYZ,BZ,NBZ,C,NX,XB,YB,IMK)		2040
	IF (IDBUG .NE. 0) WRITE(6,970) (XB(I),YB(I), I=1,NX)		2050
	IF (IMK .EQ. 0) GO TO 130		2060
C			2070
C	CONTOURS FOR KONTUR = 2 OR 3		2080
C			2090
	ISKIP = 1		2100
	NEAR = 0		2110
	ICT = 0		2120
	DO 120 IY = 1,NT		2130
	CALL FUN23(IY,IMK,NP,ND,U,V,IER)		2140
	IF (IER .NE. 0) GO TO 500		2150
	CALL SCALUV(IY,V,ND)		2160
	CALL COORD(U,V,ND,C,XC,XX,YY)		2170
	IF (IDBUG .NE. 0) WRITE(6,940) C,XC,(U(I),V(I), I=1,ND)		2180
	IF (XC .LT. -1.E60) GO TO 120		2190
	ICT = ICT+1		2200

	X(ICT) = XC	2210
	Y(ICY) = TG(IY)	2220
120	CONTINUE	2230
	IF (IMK .EQ. 2) CALL XTENT(IFLG,NT,ICT,X,Y,C,XX,YY)	2240
	CALL SERT(IMK,X,Y,ICT,XB,YB,NX,IER)	2250
	IF (IER .NE. 0) GO TO 500	2260
	IF (ICT .LT. 3) GO TO 210	2270
	CALL SCALXY(X,Y,ICT)	2280
	IK = 0	2290
	IF (IDBUG .NE. 0) WRITE(6,940) (X(I),Y(I),I=1,ICT)	2300
	NCPLT = NCPLT+1	2310
	CPLT(NCPLT) = C	2320
	IF (IMK .EQ. 2) GO TO 125	2330
	ISKIP = 0	2340
	NEAR = 0	2350
	CALL FLINE(X,Y,-ICT,1,0,0,XX,YY)	2360
	CALL GRAPH(IK,XX,YY,-6)	2370
	CALL MARK(XX,YY,IK,XB,YB,NX,IMK,C)	2380
	GO TO 210	2390
125	CALL MARK(X,Y,ICT,XB,YB,NX,IMK,C)	2400
	IF (NX .NE. 1) GO TO 126	2410
	CALL FLINE(X,Y,-ICT,1,ICT-1,IMK,XX,YY)	2420
	GO TO 210	2430
126	CALL ENTHAL(X,Y,ICT,XB,YB,NX,XX,YY)	2440
	GO TO 210	2450
130	ICT = 0	2460
	ISKIP = 1	2470
	NEAR = 0	2480
	IF (NX .NE. 2) GO TO 170	2490
C		2500
C	LEFT SIDE CONTOUR, FUNCTION 1	2510
C		2520
	DO 140 IY = 1,NT	2530
	IF (TG(IY) .GT. YB(1)) GO TO 140	2540
	CALL FUN1(1,IY,NP,ND,U,V)	2550
	CALL SCALUV(U,V,ND)	2560
	CALL COORD(U,V,ND,C,XC,XX,YY)	2570
	IF (IDBUG .NE. 0) WRITE(6,940) C,XC,(U(I),V(I),I=1,ND)	2580
	IF (XC .LT. -1.E60) GO TO 140	2590
	ICT = ICT+1	2600
	X(ICT) = XC	2610
	Y(ICY) = TG(IY)	2620
140	CONTINUE	2630
	ICT = ICT+1	2640
	X(ICY) = XB(1)	2650
	Y(ICY) = YB(1)	2660
	IF (ICT .LT. 3) GO TO 145	2670
	CALL SCALXY(X,Y,ICT)	2680
	IK = 0	2690
	IF (IDBUG .NE. 0) WRITE(6,940) (X(I),Y(I),I=1,ICT)	2700
	CALL FLINE(X,Y,-ICT,1,ICT-1,IMK,XX,YY)	2710
C		2720
C	RIGHT SIDE, FUNCTION 1	2730
C		2740
145	X1 = XB(2)	2750

	Y1 = YB(2)	2760
150	ICT = 1	2770
	X(1) = X1	2780
	Y(1) = Y1	2790
	DO 160 IY = 1,NT	2800
	IF (TG(IY) .LT. Y1) GO TO 160	2810
	CALL FUN1(2,IY,NP,ND,U,V)	2820
	CALL SCALUV(U,V,ND)	2830
	CALL COORD(U,V,ND,C,XC,XX,YY)	2840
	IF (IDBUG .NE. 0) WRITE(6,940) C,XC,(U(1),V(1),I=1,ND)	2850
	IF (XC .LT. -1.E60) GO TO 160	2860
	ICT = ICT+1	2870
	X(ICT) = XC	2880
	Y(ICT) = TG(IY)	2890
160	CONTINUE	2900
	IF (ICT .LT. 3) GO TO 165	2910
	CALL SCALXY(X,Y,ICT)	2920
	IK = 0	2930
	IF (IDBUG .NE. 0) WRITE(6,940) (X(I),Y(I),I=1,ICT)	2940
	NCPLT = NCPLT+1	2950
	CPLT(NCPLT) = C	2960
	CALL FLINE(X,Y,-ICT,1,ICT-1,IMK,XX,YY)	2970
165	IF (NX .EQ. 2) CALL GRAPH(2,XB,YB,0)	2980
	CALL MARK(XX,YY,IK,XB,YB,NX,IMK,C)	2990
	GO TO 210	3000
170	IF (NX .EQ. 1) GO TO 200	3010
C		3020
C	FUNCTION 1 WITH NO INTERSECTIONS	3030
C		3040
	ICT = 0	3050
	DO 180 IP = 1,2	3060
	DO 180 IY = 1,NT	3070
	IF (IP .EQ. 1 .AND. TG(IY) .GT. YBIG) GO TO 180	3080
	CALL FUN1(IP,IY,NP,ND,U,V)	3090
	CALL SCALXY(U,V,ND)	3100
	CALL SCALU(U,V,ND)	3110
	CALL COORD(U,V,ND,C,XC,XX,YY)	3120
	IF (IDBUG .NE. 0) WRITE(6,940) C,XC,(U(1),V(1),I=1,ND)	3130
	IF (XC .LT. -1.E60) GO TO 180	3140
	ICT = ICT+1	3150
	X(ICT) = XC	3160
	Y(ICT) = TG(IY)	3170
180	CONTINUE	3180
	IF (ICT .LT. 3) GO TO 210	3190
	CALL SCALXY(X,Y,ICT)	3200
	IK = 0	3210
	IF (IDBUG .NE. 0) WRITE(6,940) (X(I),Y(I),I=1,ICT)	3220
	NCPLT = NCPLT+1	3230
	CPLT(NCPLT) = C	3240
	CALL FLINE(X,Y,-ICT,1,ICT-1,IMK,XX,YY)	3250
	CALL MARK(XX,YY,IK,XB,YB,NX,IMK,C)	3260
	GO TO 210	3270
C		3280
C	FUNCTION 1 WITH ONE INTERSECTION (RIGHT SIDE)	3290
C		3300

200	ICT	= 0	3310
	X1	= XB(1)	3320
	Y1	= YB(1)	3330
			3340
	GO TO 150		3350
210	CONTINUE		3360
	IF (NCPLT .GT. 0) WRITE(6,980) KONTUR,(CPLT(I),I=1,NCPLT)		3370
	GO TO 100		3380
500	IF (IER .EQ. 0) RETURN		3390
	WRITE(6,920) IER		3400
510	CALL GRAPHF		3410
	CALL EXIT		3420
	END		

C	SUBROUTINE XTENT(IFLG,NT,ICT,X,Y,C,XX,YY)	10
C		20
C	PURPOSE	30
C		40
C	X,Y ARE ICT PAIRS OF COORDINATES FOR ISENTHALP, C.	50
C	XX,YY ARE INCLUDED TO PASS THE LOCATION OF THESE ARRAYS TO	60
C	OTHER SUBROUTINES.	70
C		80
C	NT IS THE NUMBER OF TEMPERATURES IN THE SOURCE DATA GRID.	90
C	IFLG IS NOT USED. ON RETURN, X,Y WILL INCLUDE COORDINATES FOR C	100
C	OBTAINED FROM THE PRESSURE GRID DATA.	110
C		120
C		130
C	SUBROUTINES CALLED	140
C	SCALUV, COORD	150
C		160
C	REVISED 720307 TO INCLUDE ALL GIVEN PRESSURE DATA.	170
C		180
C	COMMON DB(R00),TG(50),PG(50),RE(50,8),Z1301(2700),RG(50,50,3)	190
C		200
C	DIMENSION X(1),Y(1),XX(1),YY(1),XP(52),YP(52),GT(52)	210
C		220
	NP = DB(13)	230
	DO 60 J = 1, NP	240
	JP = 0	250
	DO 10 I = 1, NT	260
	IF (RG(I,J,3) .EQ. 0.) GO TO 10	270
	BPR = -1.E70	280
	IF (RE(I,8) .NE. 0.) BPR=RE(I,8)	290
	IF (RG(I,J,3) .LT. BPR) GO TO 10	300
	JP = JP+1	310
	GT(JP) = TG(I)	320
	XP(JP) = RG(I,J,3)	330
	YP(JP) = RG(I,J,2)	340
		350
10	CONTINUE	360
	CALL SCALUV(GT,YP,JP)	370
	CALL COORD(GT,YP,JP,C,YC,XX,YY)	380
	IF (YC .LT. -1.E60) GO TO 60	390
	CALL SCALUV(XP,GT,JP)	400
	CALL COORD(XP,GT,JP,YC,XC,XX,YY)	410
	IF (XC .LT. -1.E60) GO TO 60	420
	I = 0	430
20	I = I+1	440
	IF (I .GT. ICT) GO TO 50	450
	IF (XC .LE. X(1)) GO TO 22	460
	L = 1	470
	GO TO 25	480
22	L = I+1	490
	IF (L .GT. ICT) GO TO 50	500
	IF (XC .GE. X(L-1) .OR. XC .LE. X(L)) GO TO 20	510
	IF (YC .LE. Y(L-1) .OR. YC .GE. Y(L)) GO TO 60	520
25	DO 30 K = L, ICT	530
	K1 = ICT+L-K	540
	X(K1+1) = X(K1)	550


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30      Y(K1+1) = Y(K1)
        X(L)   = XC
        Y(L)   = YC
        ICT    = ICT+1
50      GO TO 60
        ICT    = ICT+1
        X(ICT) = XC
        Y(ICT) = YC
60      CONTINUE
        RETURN
        END

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C	SUBROUTINE YSECT (IBIG,BXY,BY,NBY,BYZ,BZ,NBZ,C,NX,XB,YB,IMK)	10
C		20
C	PURPOSE	30
C		40
C	YSECT LOCATES ANY INTERSECTIONS OF CONTOUR C WITH THE SATURATION	50
C	CURVE. THE NX SUCH INTERSECTIONS HAVE COORDINATES STORED INTO	60
C	XB,YB.	70
C		80
C		90
C	DIMENSION BXY(1),BY(1),BYZ(1),BZ(1),XB(1),YB(1),IBIG(1)	100
C		110
	NX = 0	120
	J = 1	130
	IMAX = IBIG(1)	140
	ILIM = IBIG(2)	150
	IX = 1	160
	I = 1	170
	IF (IMK .GT. 0) GO TO 70	180
10	I = I+1	190
	IF (I .GT. ILIM) GO TO 70	200
	D1 = C-BZ(I-1)	210
	D2 = C-BZ(I)	220
	IF (D1*D2 .GT. 0.) GO TO 10	230
	NX = NX+1	240
	IF (NX .LE. 2) GO TO 20	250
	XB(1) = XB(2)	260
	YB(1) = YB(2)	270
	NX = 2	280
20	D1PD2 = ABS(D1)*ABS(D2)	290
	IF (D1PD2 .NE. 0.) GO TO 25	300
	V = BYZ(I-1)	310
	GO TO 30	320
25	DD = ABS(D1)/D1PD2	330
	V = DD*(BYZ(I)-BYZ(I-1))+BYZ(I-1)	340
30	YB(NX) = V	350
40	IX = IX+1	360
	IF (IX .GT. IMAX) GO TO 85	370
	D1 = V-BY(IX-1)	380
	D2 = V-BY(IX)	390
	IF (D1*D2 .GT. 0.) GO TO 40	400
50	D1PD2 = ABS(D1)*ABS(D2)	410
	IF (D1PD2 .NE. 0.) GO TO 55	420
	U = BXY(IX-1)	430
	GO TO 60	440
55	DD = ABS(D1)/D1PD2	450
	U = DD*(BXY(IX)-BXY(IX-1))+BXY(IX-1)	460
60	XB(NX) = U	470
	I = I+1	480
	GO TO 10	490
70	IF (J .EQ. 2) GO TO 80	500
	J = 2	510
	I = ILIM+1	520
	IX = IMAX+1	530
	IMAX = NBY	540
		550

	ILIM = NBZ	560
	GO TO 10	570
A0	RETURN	580
85	WRITE(6,910) C,(XB(K),YB(K),K=1,NX)	590
910	FORMAT(1H0,'NO MATCHING XB. C AND XB,YB ARE: ',1X,SE15.6//)	600
	CALL GRAPHE	610
	CALL EXIT	620
	END	630

8. PROPRIETARY SUBROUTINES CALLED

Monsanto subroutines

1. GRAPH
2. GRAPHE
3. GRAPHI

(These are entry points in the same subroutine, GRAPHE.)

CalComp subroutines

1. FIT4
2. FLINE
3. NUMBER
4. PLOT
5. REFLX
6. SYMBOL
7. WHERE

Note: The complete set of routines in the "CalComp Basic Software Package" is used either directly or indirectly. Items 1, 2, and 5, above, are modified from those in the "Scientific Applications" category of CalComp's "Functional Software Library"; they are not included with the Basic Software.

8.1 Monsanto Subroutines

Uses and arguments of each are described below along with the format of the call statements. Any numerical values given in the argument list pertain only to specific options provided by the Monsanto routines. Arguments shown by name are the only ones passing information essential for TSPLLOT. Section 2.2.1 of the program description and the listing of TSPLLOT also define these arguments.

The subroutines use the CalComp Basic Software package.

(a) CALL GRAPHI (0,-1,SCALES,1,TITLE,1,AXISID,0,0,0,0)

SCALES is an array of size 6 containing the axis scaling data.

TITLE is an array of size 18 containing 72 characters for the plot title.

AXISID is an array of size 18 containing 72 characters, 36 each for X and Y axes labels

A call to GRAPHI places data on the plot tape for plotting the title.

(b) CALL GRAPH (N,X,Y, IT)

- N is the number of data points in array X (and Y).
- X is an array of size greater than or equal to $N + 2$. X contains the X-axis values in the first N locations. On return from GRAPH, X (N + 1) will contain the X-value at the origin of the plot and X (N + 2) will contain the units per inch for the X-axis.
- Y is an array of size greater than or equal to $N + 2$. Y contains the Y-axis values in the first N locations. On return from GRAPH, Y(N + 1) will contain the Y-value at the origin of the plot and Y(N + 2) will contain the units per inch for the Y-axis.
- IT is an integer code to specify how the line is to be plotted.
- IT = 0 for continuous line through the data points.
- IT < -1 is used to produce a dashed line. Points 1 to $i + IT - 1$ are connected by straight line segments if, and only if, $(i + IT - 2) / (IT - 1)$ is an odd integer.

Calls to GRAPH are used to complete the plot border, to plot dashed lines for density contours, and to place tic marks where enthalpy contours intersect the liquid side of the two phase boundary.

(c) CALL GRAPHE

No arguments are used with GRAPHE. It is used to write a record on the plot tape which indicates the end of the plot data. When no more plots are to be made, program E1393 makes a call to GRAPHE.

8.2 CalComp Subroutines

(a) FIT4

FLINE calls FIT4 which calculates points for a smooth curve.

(b) FLINE

This routine plots a smooth curve through a given set of data points using a modified spline technique. Changes have been made to the original CalComp version so that arrays of the coordinates used for plotting are returned to the calling program.

(c) NUMBER

NUMBER converts a floating-point number to the appropriate decimal equivalent so that the number may be plotted in Fortran F-type format.

(d) PLOT

PLOT generates the actual plotter commands.

(e) REFLX

REFLX is called by FLINE to handle end conditions for the spline-fitted curve.

(f) SYMBOL

SYMBOL is used to draw annotation (titles, labels, etc.).

(g) WHERE

WHERE is an entry point in PLOT which returns current pen coordinates.

APPENDIX N

FLASH AND FIRE POINTS, MICRO-CLEVELAND OPEN CUP METHODS

To obtain these measurements a modified Cleveland open cup apparatus was employed in a procedure approximate to that described in ASTM D-92. Exceptions to the ASTM method, adopted to permit measurements when sample sizes are greatly limited by cost or availability, were as follows:

1. Cup external measurements are standard, but the sample well was reduced to a hole 1.25 in. diam. x 1.25 in. deep and the sample size was 18-20 cc.
2. The well was fitted with a glass dome (as a cover) supported by the ASTM flash point thermometer, which in turn was supported on-axis with the sample well.
3. To test for flash/fire point, the thermometer-dome assembly were lifted off the cup to permit the normal traverse of the pilot flame over the liquid surface at each 5°F. interval.

The flash and fire points were recorded as specified in ASTM D-92.

APPENDIX O

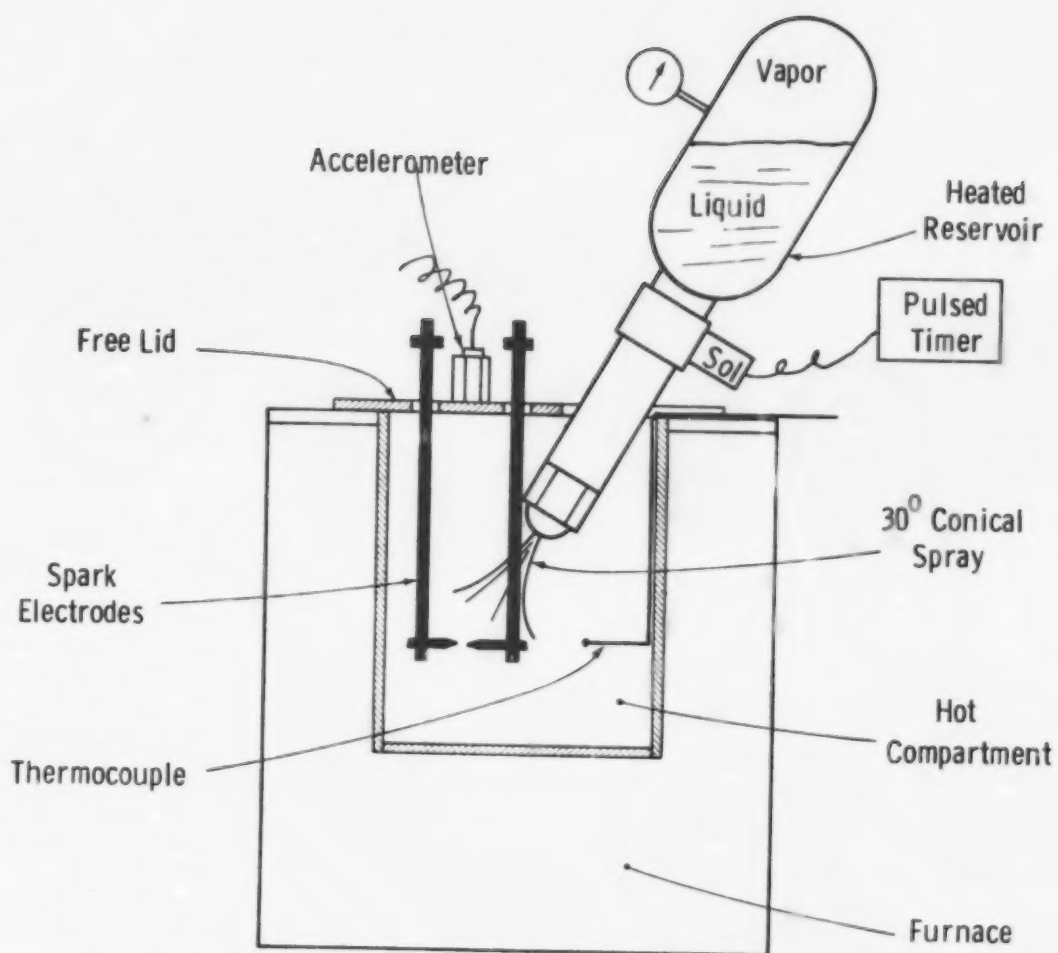
THE HOT COMPARTMENT SPRAY IGNITION TEST

The apparatus is constructed to represent a spray from a system containing a liquid at elevated temperature and pressure into a controlled temperature air environment having a high temperature ignition source. The apparatus, illustrated in Figure O-1, contains a closed reservoir which is filled with 30 cc of working fluid and heated to the desired equilibrium temperature and pressure. A solenoid valve is triggered for a fixed time interval allowing fluid to spray through a 60° cone angle hollow spray nozzle having the following flow characteristics with water at room temperature:

<u>Reservoir Pressure (psi)</u>	<u>Volume Flow Rate (cc/min)</u>
200	103
400	130
600	166
800	166
1000	187

The spray is aimed at a 10,000 volt, 1/8 gap spark at a distance of 2 inches in a controlled temperature chamber (5 in. dia. x 5 in. long).

The test procedure is to start the bomb filled with 30 cc of working fluid at a pressure of 1000 psig and spray into the 100°C chamber for 1/4 second. The spark source is started two seconds before the spray and remains on for the duration of the test. A relative maximum average explosive peak force is measured using a meter reading of the dc amplitude from the accelerometer attached to the bomb cover. The compartment temperature rise is measured with a fine wire-thin wall jacketed thermocouple. The existence and duration of flash and fire are determined visually.



MONSANTO HOT COMPARTMENT IGNITION TEST

Spray Time - 1/4 sec.

Compartment Temp. - 100°C

Initial Fluid Charge - 30cc

Compartment Environment - Air

Figure O-1. Monsanto Hot Compartment Ignition Test

APPENDIX P

MONSANTO RECORDING TENSIMETER

For vapor pressure measurements the fluid samples are charged to a sample cell which is placed in a heated environment. The sample oven with its associated temperature controller comprised a bench-top unit; the recorder and electronic components were mounted in a floor cabinet. Figure P-1 shows a diagram of the tensimeter.

The oven and programmer assembly were the corresponding components of a Perkin-Elmer Model F-11 gas chromatograph. An insulated top was made for the oven, occupying the space where the chromatograph detector normally would have been placed. The top was secured only by gravity so that in case of an explosion of the sample cell internal pressure in the oven would be relieved by lifting of the top. The base of the oven unit contained the temperature control electronics. The base front panel originally had oven temperature and injection temperature controls and a heater switch; a new panel was made, eliminating those controls which were not required for the tensimeter application. A hole was cut in the front wall of the oven to admit the sample cell.

The recorder used with the apparatus was a Hewlett-Packard Model 7035A, an inexpensive x-y recorder without time base. It was modified to have a single, fixed range on the 254 mm axis (which would be the pressure axis of the chart), and three ranges on the 178 mm axis (the temperature axis). The recorder panel provided a mounting also for the $\log p - \log \Delta p/\Delta t$ function switch, which actually had no connection with the recorder circuits. The recorder was mounted in the inclined upper-panel space of a cabinet 1.3 m high, with the auxiliary components in three drawers below; electronic circuits for temperature and pressure measurement in the top, timers for the decomposition-rate system in the middle, and power supplied in the bottom.

The specifications of the instrument were as follows:

Oven assembly -

Temperature range: room - 500°C

Cut-off temperature of programmer: selectable to 500°C

Safety cut-off temperature: approximately 480°C not adjustable

Programming rate: 1, 1.5, 2, 3, 4, 5, 6, 8, 10, 12, 15, 18, 20, 25, 30 and 40°C per minute

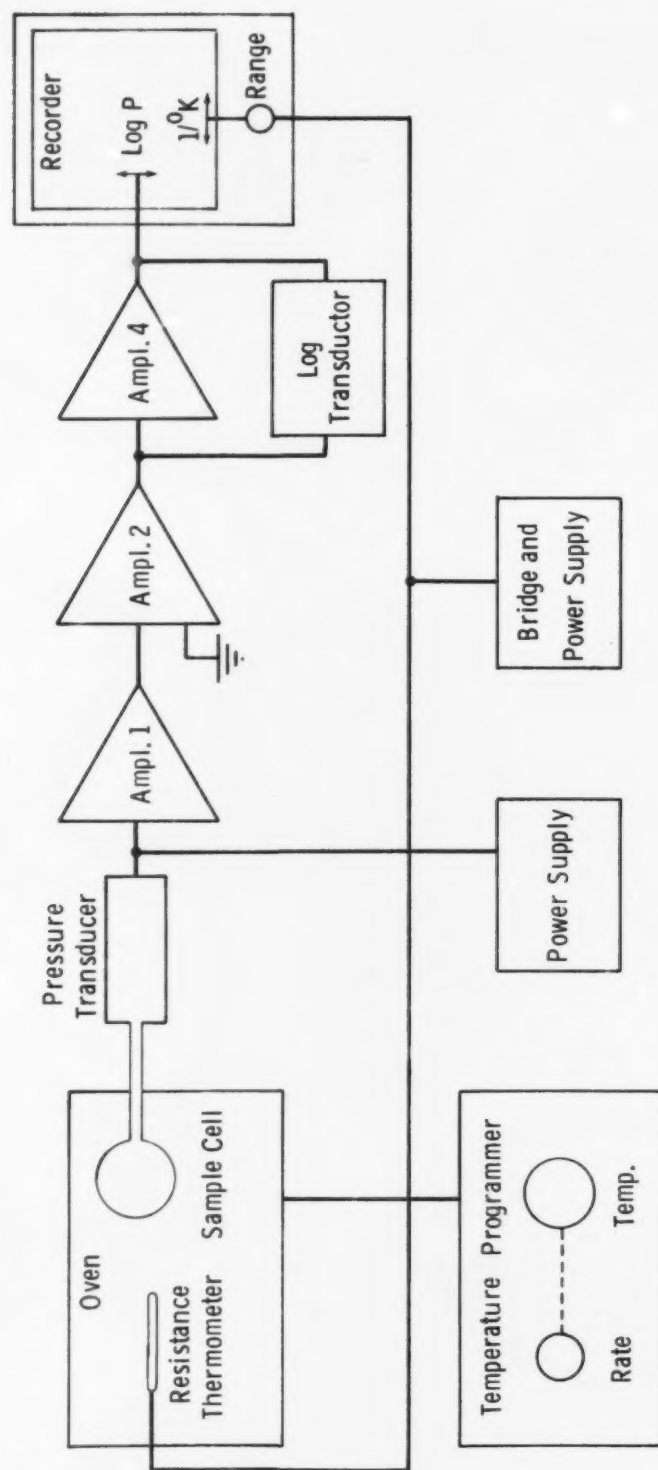


Figure P-1. Monsanto Recording Tensimeter

Log p recording system -

Pressure range: 10 - 1000 torr

Log $\Delta p/\Delta t$ recording system -

Pressure range: 1 - 100 torr increase of pressure within the recording interval

Programmer temperature advance interval: 60 sec (selectable 2-60 sec)

Hold interval: 300 sec (selectable 60-1800 sec)

Recording interval: 144 sec (selectable 10-300 sec)

Temperature recording system -

Ranges: 0-500°C, 0-150°C and 150-500°C, presented on scales linear in 1/°K

The initial modification to the instrument was the adapting a stainless steel tubular sample cell and high pressure transducer to measure vapor pressures of the working fluids. The total cell volume is 5.75 cc. When a 4 cc sample is charged to the cell, the volume heated by the oven is 2.25 cc.

APPENDIX Q

FIXED CYCLE COMPUTATIONS

In order to evaluate the Rankine cycle applicability of the fluids which passed thermal stability and I-factor screening, cycle efficiencies and other pertinent performance parameters were calculated. Two standard cycles were calculated, identified as the "Ideal Reference Cycle" (R2) and the "Equivalent Real Cycle" (R4). The cycle descriptions and computation procedures are described in the following paragraphs.

1. CALCULATION PROCEDURE - REFERENCE IDEAL CYCLE (R2)

1.1 Description of Cycle

(See Figure Q-1. Letters in parentheses refer to points on the diagram.)

- (1) Pump inlet conditions are set as saturated liquid at 220°F (E).
- (2) Expander inlet conditions are set at 712°F (A). The pressure is chosen as the maximum pressure, not greater than 1000 psia, from which an isentropic expansion to the pump inlet pressure can be made without producing condensation anywhere in the expander.
- (3) Expansion is isentropic from expander inlet to pump inlet pressure (B).
- (4) Expander exit gases are cooled in a regenerator at constant pressure to a saturated vapor condition (C).
- (5) Condensation at constant pressure is allowed in the regenerator until heat is transferred sufficient to raise the temperature of the liquid side of the regenerator from the pump exit temperature to the saturated vapor temperature (D).
- (6) The vapor-liquid mixture then enters the condenser where it is totally condensed at constant pressure to pump inlet conditions (E).
- (7) The liquid is pumped isentropically to the expander inlet pressure (F).

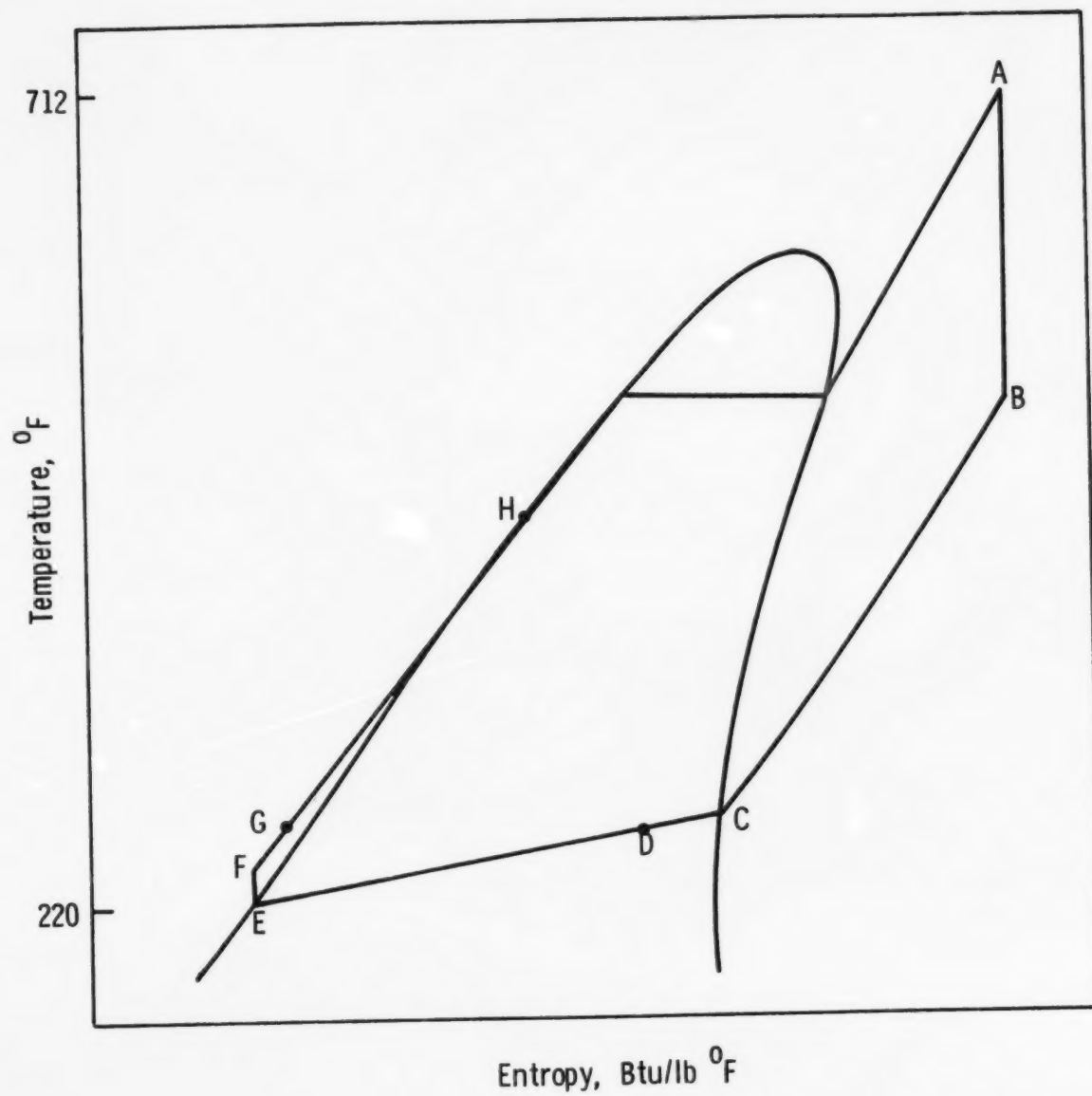


Figure Q-1. Reference Ideal Cycle

- (8) The liquid passes through the regenerator at constant pressure, recovering first the partial condensation heat from the vapors (G) and then the sensible heat (H).
- (9) The fluid then passes through the vapor generator where it is heated at constant pressure to the expander inlet conditions (A).

1.2 Computation Details

The preliminary calculations consist of determining the properties (pressure, temperature, enthalpy, entropy, density) at each reference point (A through H) on the cycle diagram. The steps in this procedure are as follows:

- (1) Obtain a standard set of tables from program E-1393 giving saturated liquid and saturated vapor tables, and single phase tabulations. Temperatures in the tables are at 20°F increments from 180°F to 800°F. Pressures calculated are 10, 14.696, 25, 50, 100, 200, 300, 500, 700, 900 and 1000 psia.
- (2) The properties at point E are read directly from the tables for saturated liquid at 220°F.
- (3) E-1393 is used again to produce an isobar at the pressure P_E . The properties of point C are read directly from the saturated vapor table of this set.
- (4) The saturated vapor tables are then scanned to determine the maximum entropy, S_{max} , between point C and the critical point.
- (5) The entropy at 1000 psia and 712°F, S_{1000} , is determined by interpolation from the 1000 psia isobar tables. If this value is greater than S_{max} , the coordinates of point A are established as 712°F, 1000 psia. If $S_{1000} < S_{max}$, entropies at 712°F are obtained from the various isobars, plotted vs. pressure, and the pressure having $S = S_{max}$ is established as P_A . E-1393 is again used to obtain an isobar at P_A . Other properties are read from the tables along the P_A isobar. In almost every case 1000 psia was chosen as P_A .
- (6) P_B is taken as P_E . T_B and other properties are found by interpolating in the tables for the P_E isobar such that $S_B = S_A$.

- (7) Point F is established by setting $P_F = P_A$, and interpolating in the P_A isobar tables to set $S_F = S_E$.
- (8) Point G is established by setting $P_G = P_A$, and $T_G = T_C$.
- (9) Point D is established by setting $P_D = P_A$, and $H_D = H_C + H_F - H_G$.
- (10) Point H is established by setting $P_H = P_A$, and $H_H = H_G + H_B - H_C$.

After the reference point properties have been determined, the performance calculations are made as follows:

Efficiencies:

Carnot - Set by the chosen maximum and minimum temperatures to be 42%.

$$\text{Cycle, 0\% Regen: } E = 100 \frac{H_A - H_B - (H_F - H_E)}{H_A - H_H}$$

$$\text{Cycle, 100\% Regen: } E = 100 \frac{H_A - H_B - (H_F - H_E)}{H_A - H_H}$$

Cycle: $E = (\text{Cycle, 100\% Regen})$ or
 $E = 30\%$, whichever is less
 % of Carnot: $100 \times \text{cycle efficiency} / 42$

Temperatures:

MaxF = 712°F
 MinF = 220°F

Pressures:

Max psia = P_A
 Min psia = P_E

Per 100 Net Cycle Horse Power:

$$\text{Fluid rate, lb/hr: } \frac{100 \times 2545.08}{H_A - H_B - (H_F - H_E)}$$

$$\text{Engine exhaust, cfm: } \frac{\text{Fluid Rate}}{\rho_B \times 60}$$

$$\text{Pump In, gpm: } \frac{\text{Fluid Rate} \times 7.48}{\rho_E \times 60}$$

$$\text{Engine HP, gross: } 100 \frac{H_A - H_B}{H_A - H_B - (H_F - H_E)}$$

$$\text{Pump HP: Engine HP, gross} - 100$$

Heat Flows:

If cycle efficiency is set at 30%, points H and D are adjusted as follows:

$$H_{H'} = H_A - \frac{H_A - H_B - (H_F - H_E)}{0.3}$$

$$H_{D'} = H_D + H_H - H_{H'}$$

Other properties are interpolated at P_H and P_D respectively.

$$\text{Heater, KBtu/hr } \frac{\text{Fluid Rate} \times (H_A - H_{H'})}{1000}$$

$$\text{Regen, KBtu/hr } \frac{\text{Fluid Rate} \times (H_B - H_{D'})}{1000}$$

$$\text{Cond, KBtu/hr } \frac{\text{Fluid Rate} \times (H_{D'} - H_E)}{1000}$$

Without Regen:

Add Regen, KBtu/hr to Heater, KBtu/hr, and to Cond, KBtu/hr

Engine:

% Eff.: Set at 100%

Pressure Ratio: P_A/P_B

Density Ratio: ρ_A/ρ_B

$$\text{Exhaust Quality, \%: } 100 \frac{H_B - H_E}{H_C - H_E}$$

$$\text{Delta H, Btu/lb: } H_A - H_B$$

Nozzles:

Coeff: Set at 1.00

$$V_{\text{spout}}, \text{ FPS: } 223.72 \sqrt{H_A - H_B}$$

$$\text{Mach. No. Spout: } \frac{V_{\text{spout}}}{C}$$

$$\text{where } C = 68.062 \left(\frac{\partial p}{\partial \rho} \right)_{S_B}^{0.5}$$

$$\left(\frac{\partial p}{\partial \rho} \right)_{S_B} \text{ is obtained graphically from the thermodynamic tables}$$

$$A_{\text{throat}}: \frac{.04 \times \text{Fluid Rate}}{\rho_{\text{throat}} C}$$

$$\text{where } S_{\text{throat}} = S_A$$

$$H_{\text{throat}} = H_A - \left(\frac{C}{223.72} \right)^2$$

Regenerator: (for 30% cycle efficiency)

$$\% \text{ Effective: } \frac{H_{H'} - H_F}{H_H - H_F} \times 100$$

Q, KBtu/hr: Calculated under "Heat Flows"

$$UA: \frac{Q}{\Delta T_{LM}}$$

ΔT_{LM} : Non-condensing regenerator

$$\frac{(T_B - T_H) - (T_C - T_F)}{\ln \left(\frac{T_B - T_H}{T_C - T_F} \right)}$$

A single ΔT_{LM} cannot be calculated for a condensing regenerator

$$NTU_{(OG)}: \frac{T_B - T_C}{\Delta T_{LM}}$$

$$I_{\text{factor at } 220^\circ\text{F}}: I = \frac{RT}{C_p} \frac{dP}{dT}$$

where $\frac{dP}{dT}$ is the slope of the P vs T plot along the saturated vapor curve (obtained graphically) at 220°F , and

$$C_p = \left(\frac{\partial H}{\partial T} \right)_p$$

evaluated graphically at $P = P_B$

2. CALCULATION PROCEDURE - EQUIVALENT REAL CYCLE (R4)

2.1 Description of Cycle

(See Figure Q-2. Letters in parentheses refer to points on the diagram.)

- (1) Pump inlet conditions are set as saturated liquid at 220°F (E).
- (2) Expander inlet conditions are set at 712°F (A). The pressure is chosen as the maximum pressure, not greater than 1000 psia, from which an isentropic expansion to the pump inlet pressure can be made without producing any condensation in the expander.

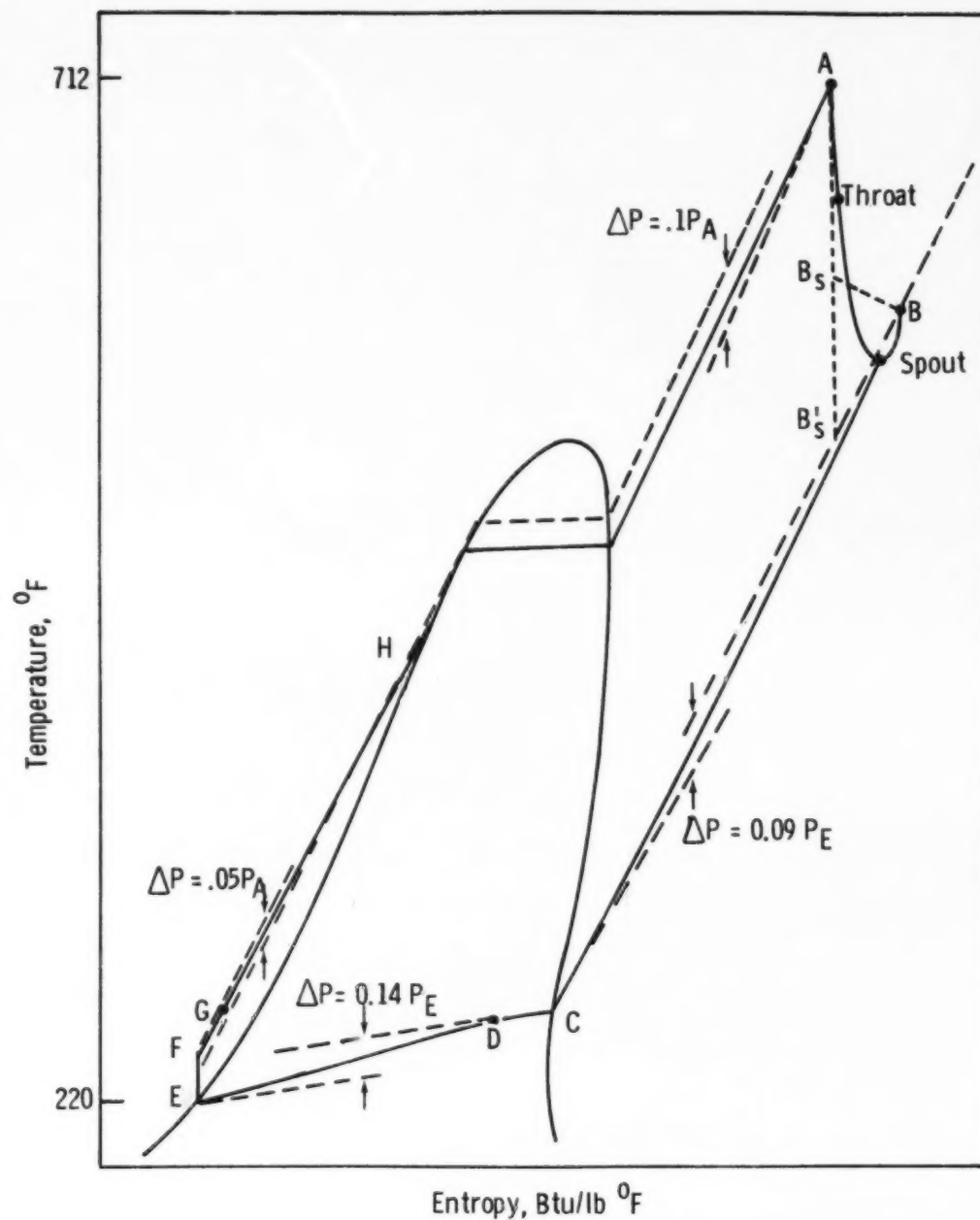


Figure Q-2. Equivalent Real Cycle

- (3) Expansion follows the curved path (A) to (throat) to (spout) to (B). Properties are approximated by an isentropic expansion to (B_s) giving 75% expander efficiency, followed by an isenthalpic expansion to (B).
- (4) Expander exit gases are cooled in a regenerator to a saturated vapor (C) with a pressure drop 9% of pump inlet pressure.
- (5) Condensation at constant pressure is allowed until the capacity of a heat exchanger of $UA_k = 125 \text{ Btu/HP-hr-}^\circ\text{F}$ is used (D).
- (6) The vapor-liquid mixture is totally condensed with a pressure drop 14% of pump inlet pressure, to the pump inlet (E).
- (7) The liquid is pumped isentropically (but with a 75% efficient pump) to the liquid side regenerator pressure (F).
- (8) The liquid passes through the regenerator with a pressure drop 5% of expander inlet pressure recovering first the partial condensation heat from the vapors (G) and then the sensible heat (H).
- (9) The fluid then passes through the vapor generator with pressure drop 10% of expander inlet pressure to the expander inlet conditions (A).

2.2 Computation Details

Preliminary calculations consist of determining the properties (pressure, temperature, enthalpy, entropy, density) at each reference point (A through H, B_s , $B_{s'}$, throat and spout) on the cycle diagram. The steps in this procedure are as follows:

- (1) Obtain a standard set of tables from program E-1393 giving saturated liquid and saturated vapor tables, and single phase tabulations. Temperatures in the tables are at 20°F increments from 180°F to 800°F . Pressures calculated are 10, 14.696, 25, 50, 100, 200, 300, 500, 700, 900, 1000, 1100 and 1150 psia.
- (2) Point E properties are read directly from saturated liquid tables at 220°F .
- (3) E-1393 is used again to produce isobars at P_E 1.14 P_E . Point C properties are read directly from the saturated vapor properties at 1.14 P_E .

- (4) The saturated vapor tables are then scanned to determine the maximum entropy, $S_{\max}$, between point C and the critical point.
- (5) The entropy at 1000 psia and 712°F, S_{1000} , is determined by interpolation from the 1000 psia isobar tables. If this value is greater than $S_{\max}$, the coordinates of point are established as 712°F, 1000 psia.

If $S_{1000} < S_{\max}$, entropies at 712°F are obtained from the various isobars, plotted vs pressure, and the pressure having $S = S_{\max}$ is established as P_A . E-1393 is again used to produce tables at P_A , $1.1 P_A$, and $1.15 P_A$. Other properties for point A are read from the tables along the P_A isobar.

- (6) $P_{B's}$ is taken as $1.23 P_E$. $S_{B's} = S_A$, and other properties interpolated on the $1.23 P_E$ isobar.
- (7) $S_{Bs} = S_A$. $H_{Bs} = H_A - 0.75(H_A - H_{Bs})$. Other properties interpolated from tables.
- (8) $H_B = H_{Bs}$. $P_B = 1.23 P_E$. Other properties interpolated from tables.
- (9) $P_{\text{spout}} = P_B$. T_{spout} is obtained by trial and error to obtain

$$P_{\text{spout}} v_{\text{spout}} = 0.95 P_{B's} v_{B's}$$

where $v_{B's} = 223.72 \sqrt{H_A - H_{B's}}$

$$v_{\text{spout}} = 223.72 \sqrt{H_A - H_{\text{spout}}}$$

- (10) $S_{\text{throat}} = S_A + 0.25 (S_B - S_A)$
Obtain C, speed of sound graphically, as

$$C = 68.062 \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_{S_{\text{throat}}}}$$

by plotting P vs ρ at $S = S_{\text{throat}}$

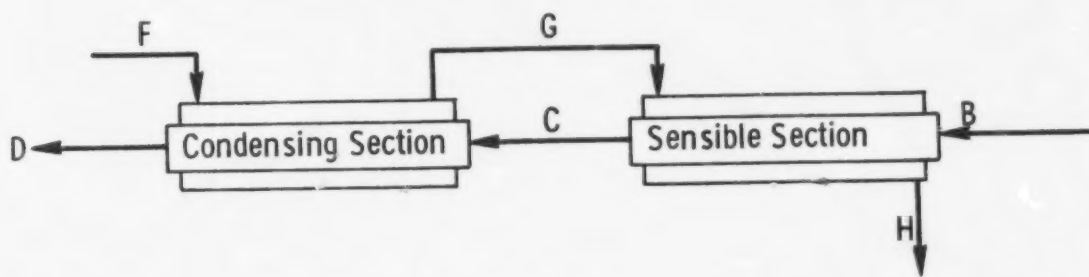
Then:

$$H_{\text{throat}} = H_A - \left(\frac{C}{223.72} \right)^2$$

- (11) $S_F = S_E$. $P_F = 1.15 P_A$. Other properties interpolated from tables.
- (12) Points D, G and H are determined from a trial and error heat exchanger calculation. The pressures are established:

$$P_D = 1.14 P_E; P_G = 1.15 P_A; P_H = 1.1 P_A$$

The heat exchanger is conceptually broken into two sections as shown below, schematically:



T_B , T_C , and T_F are known. T_G is assumed to have some value less than T_C .

Then the corresponding H_G is read from the tables.

Then:

$$H_H = H_F + H_B - H_C$$

$$H_D = H_C - (H_G - H_F)$$

The corresponding temperatures are then obtained from the tables.

The fluid rate is obtained from:

$$F = \frac{100 \times 2545.08}{H_A - H_B - (H_F - H_E)/0.75}$$

The heat exchanger size is set at

$$UA = 12,500 \text{ Btu/}^\circ\text{F (100 HP)}$$

The specific size (per pound of fluid) is given by:

$$(UA)_{\text{Sp.}} = \frac{12,500}{F} \text{ Btu/}^\circ\text{F-lb}$$

For each section of heat exchanger,

$$UA = \frac{q}{\Delta T_{\text{LM}}}$$

Thus,

$$(UA)_{\text{condensing}} = \frac{(H_C - H_D) \ln \left(\frac{T_D - T_F}{T_C - T_G} \right)}{T_D - T_F - (T_C - T_G)}$$

$$(UA)_{\text{sensible}} = \frac{(H_B - H_C) \ln \left(\frac{T_B - T_H}{T_C - T_G} \right)}{T_B - T_H - (T_C - T_G)}$$

T_G is varied until:

$$(UA)_{\text{condensing}} + (UA)_{\text{sensible}} = (UA)_{\text{sp.}}$$

In the course of the calculations, T_G is set equal to T_C for one trial to determine the 100% regeneration points D' , G' and H' . For this case $UA = \infty$ and is not calculated.

After the reference point properties have been determined, the performance calculations are made as follows:

Efficiencies:

Carnot: 42%

$$\text{Cycle, 0\% Regen: } 100 \frac{H_A - H_B - (H_F - H_E)/0.75}{H_A - H_F}$$

$$\text{Cycle, 100\% Regen: } 100 \frac{H_A - H_B - (H_F - H_E)/0.75}{H_A - H_H}$$

$$\text{Cycle: } 100 \frac{H_A - H_B - (H_F - H_E)/0.75}{H_A - H_H}$$

$$\% \text{ of Carnot: } 100 \times \text{cycle efficiency}/42$$

Temperatures:

$$\text{Max F} = 712^\circ\text{F}$$

$$\text{Min F} = 220^\circ\text{F}$$

Pressures:

$$\text{Max psia} = P_F$$

$$\text{Min psia} = P_E$$

Per 100 cycle HP

Fluid rate: calculated in Preliminary Step 11.

$$\text{Engine exhaust, cfm: } \frac{\text{Fluid Rate}}{\rho_E \times 60}$$

$$\text{Pump in. gpm: } \frac{\text{Fluid rate} \times 7.48}{\rho_E \times 60}$$

$$\text{Engine HP, gross: } 100 \frac{H_A - H_B}{H_A - H_B - (H_F - H_E)/0.75}$$

$$\text{Pump HP: Engine HP, gross} - 100$$

Heat Flows:

$$\text{Heater, KBtu/hr: Fluid rate} \times (H_A - H_H)/1000$$

Regen, KBtu/hr: Fluid rate $\times (H_B - H_D)/1000$

Cond, KBtu/hr: Fluid rate $\times (H_D - H_E)/1000$

Without Regen:

Add Regen, KBtu/hr to Heater, KBtu/hr, and to Cond, KBtu/hr.

Engine:

% Eff: 75%

Pressure ratio: P_A/P_B

Density ratio: ρ_A/ρ_B

Exhaust Quality, %: $100 \frac{H_B - H_E}{H_C - H_E}$

Delta H, Btu/lb: $H_A - H_B$

Isentropic: $H_A - H_{B_S}$

Nozzles:

Coeff: 0.95

V_{spout} , fps: Calculated in preliminary step 9

Mach. No., Spout: V_{spout}/C_{spout}

where: $C_{spout} = 68.062 \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_{S_{spout}}}$

$$A_{\text{throat}}: \frac{0.04 \times \text{Fluid rate}}{\rho_{\text{throat}} C_{\text{throat}}}$$

Regenerator:

$$\% \text{ Effective: } \frac{100(H_H - H_F)}{H_{H'} - H_F}$$

Q, KBtu/hr: calculated under "Heat Flows:

UA: 12.5 KBtu/hr °F

ΔT_{LM} : Calculated for each section in preliminary step 11.

$$(NTU)_{OG}: \frac{T_B - T_C}{(\Delta T_{LM})_{\text{sensible}}} + \frac{T_C - T_D}{(\Delta T_{LM})_{\text{condensing}}}$$

I_{factor} : Same as Ideal Reference Cycle